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(57) Abstract

A three–dimensional structure is described of a complex of isopenicillin N synthase (IPNS) with Fe and its substrate ACV. This structure is used to design modified enzymes IPNS, DAOCS, DACS, DAOC/DACS and other related enzymes of the penicillin and cephalosporin biosynthesis pathway, which modified enzymes may accept unnatural substrates or improve production efficiency or produce improved products. Specific modifications of specific amino acid residues are proposed and exemplified.

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ISOPENICILLIN N SYNTHETASE AND DEACETOXYCEPHALOSPORIN C SYNTHETASE ENZYMES AND METHOD

Introduction

All commercially used penicillin and cephalosporin antibiotics and their derivatives are produced from fermentation derived materials containing a β-lactam ring. A range of organisms, including both prokaryotes and eukaryotes, and conditions may be used for their fermentation. Some are produced directly by fermentation followed by isolation. Others are produced by modification of materials produced by fermentation. Commercially used cephalosporins (also known as cephems) may be produced by modification of either fermentation derived penicillins or cephalosporins.

The biosynthetic pathway to the penicillins and cephalosporins has been extensively studied and involves the following steps (Scheme 1):

1. Three amino acids (L-α-aminoadipic acid, L-cysteine, L-valine) are condensed to form a tripeptide: L-δ-α-aminoadipoyl-L-cysteinyl-D-valine (ACV). During this process the L-valinyl residue is converted to a D-valinyl residue. This process is catalysed *in vivo* by the enzyme ACV synthetase and is common to both penicillin and cephalosporin biosynthesis.

2. ACV is converted to isopenicillin N in a step catalysed by the enzyme isopenicillin N synthase (IPNS). This step is common to both penicillin and cephalosporin biosynthesis.

3. In some organisms (*e.g. Penicillium chrysogenum* and *Aspergillus nidulans*) isopenicillin N is converted by exchange of its L-δ-α-aminoadipoyl side chain to penicillins with other side chains, which are normally more hydrophobic than the side chain of isopenicillin N. This

conversion may be catalysed by an amidohydrolase/ acyltransferase enzyme. Examples of penicillins produced by this biosynthetic process include penicillin G (which has a phenylacetyl side chain) and penicillin V (which has a phenoxyacetyl side chain). These hydrophobic penicillins may be commercially produced by fermentation under the appropriate conditions.

4. In some organisms (*e.g. Streptomyces clavuligerus* and *Cephalosporium acremonium*) isopenicillin N is epimerised to penicillin N. This reaction is catalysed by an epimerase enzyme.

5. In some organisms (*e.g. S. clavuligerus and C. acremonium*) penicillin N is converted to deacetoxycephalosporin C (DAOC). This reaction is catalysed by deacetoxycephalosporin C synthase (DAOCS) in some organisms (e.g. *Streptomyces clavuligerus*) and by deacetoxy/deacetylcephalosporin C synthase (DAOC/DACS) in others (e.g. *C.acremonium*).

6. In some organisms (e.g. *S. clavuligerus* and *C. acremonium*) DAOC is converted to deacetylcephalosporin C (DAC). This reaction is catalysed by deacetylcephalosporin C synthase (DACS) in some organisms (e.g. *S. clavuligerus*) and by deacetoxy/deacetylcephalosporin C synthase (DAOC/DACS) in others (e.g. *C. acremonium*).

Further biosynthetic steps to give other cephalosporin derivatives may also occur, e.g. in *C. acremonium* DAC may be converted to cephalosporin C and in *Streptomyces spp*. DAC may be converted to cephamycin C. The genes encoding for each of the enzymes catalysing steps 1-6 above have been identified and sequenced.

Fermented penicillins, cephalosporins, their biosynthetic intermediates, and their derivatives may be of use as antibiotics or as intermediates in the production of antibiotics. Penicillins with hydrophobic side chains may be used for the preparation of cephalosporins or intermediates used in the preparation of cephalosporins, *e.g.* penicillins

(including, but not exclusively, penicillin G and penicillin V) may be used to prepare C-3 exomethylene cephams which may be used as intermediates in the preparation of the commercial antibiotics, *e.g.* Cefachlor (Scheme 2).

For reviews see J. E. Baldwin and C. J. Schofield, in 'The Chemistry of β-lactams (Ed. M. I. Page), Chapter 1, Blackie, London 1992; Aharonowitz *et al*, Ann. Rev. Microbiol., 1992, 46, 461; Cooper, Bioorg. Med. Chem., 1993, 1, 1; Baldwin and Abraham, Nat. Prod. Report., 1989, 5, 129; Baldwin, J. Heterocyclic. Chem., 1990, 27, 91.

Summary of Invention

This invention is based on our determination of the three-dimensional structure of IPNS. That the structure of IPNS complexed to manganese has been determined, was reported by some of us in Nature, Volume 375, 22 June 1995, pages 700-704. That publication did not include the co-ordinates of the individual amino acid residues, and these are now provided. Scheme 2 of that paper contains the amino acid sequence of IPNS, and also DACS, DAOCS and DAOC/DACS and other structurally related enzymes, each of which is published in Swissprot or Genbank or other database.

We have now determined the structure of a complex of IPNS with Fe and ACV which is a substrate for the enzyme (see Scheme 1). In solution it is this complex, and not the IPNS-Mn complex, that is actually formed during step 2 of the biosynthesis of bicyclic β-lactams. Because the amino acid sequences of DAOCS, DAOC/DACS, DACS and other oxidases and oxygenases are so similar to that of IPNS, it is reasonable to expect that the structures of those enzymes are at least similar to that of IPNS.

We have also determined the structures of complexes of IPNS with Fe and with various analogues of ACV (in which another amino acid replaced L-valine), specifically AC glycine, AC aminobutyrate, AC

alanine and AC proparglyglycine. These structures have been determined in the absence and in the presence of nitrous oxide NO. Exposure of these complexes to dioxygen alters the structures, and these altered structures have also been determined by us. From information given herein about the IPNS-Fe-ACV complex, a skilled reader is able to make and characterise the other complexes referred to in this paragraph, so structural details of those other complexes are not given herein.

Thus in one aspect the invention provides Isopenicillin N synthase (IPNS) in the form of: a complex with Mn having a structure designated by the X-ray co-ordinates in Table 2; or a complex with Fe and its substrate, said complex having a structure designated by the X-ray co-ordinates in Table 3.

In another aspect the invention provides Isopenicillin N synthase (IPNS) in the form of: a complex with Fe and an analogue of its substrate, either in the absence or in the presence of nitrous oxide or dioxygen, said complex having a structure designated by X-ray co-ordinates analogous to that set out in Table 3.

An analogue of an IPNS substrate is a substrate oxidised by IPNS to give preferably (but not exclusively) a bicyclic compound containing a β-lactam ring.

Table 2 sets out co-ordinates of individual amino acid residues in a crystalline complex of IPNS with manganese.

Table 3 sets out co-ordinates of individual amino acid residues in a crystalline complex of IPNS with Fe and ACV.

Knowledge, derived from the X-ray co-ordinates, of the three-dimensional structures of this family of related enzymes permits a skilled worker to identify specific amino acids that might be changed in order to alter or improve the properties of the enzyme in some way. While it is not possible from 3D structural information alone to predict that a specific amino acid mutation will produce a specific change in the properties of the

enzyme, it is possible to identify a rather small number of amino acid residues where modification may be expected to change/improve the properties of the enzyme. The problem of identifying useful amino acid mutations is thus reduced to a level where it can readily be tackled by routine screening procedures.

Thus in one aspect the invention provides use of the three dimensional structure of a first enzyme selected from IPNS, DAOCS, DACS, DAOCS/DACS and other related enzymes of the penicillin and cephalosporin biosynthesis pathway, for the modification of a second selected from IPNS, DAOCS, DACS, DAOCS/DACS and other related enzymes of the penicillin and cephalosporin biosynthesis pathway.

The three dimensional structure of a first enzyme may be the three dimensional structure of the IPNS-Fe-substrate complex referred to above. It may, however, also be that of DAOCS, DACS, DAOC/DACS or another oxygenase/oxidase related by sequence or structure (e.g. 1-aminocylopropane-1-carboxylic acid oxidase) to any of IPNS, DAOCS, DACS or DAOC/DACS. The structure of the IPNS-Fe-ACV complex may be derived from two or more crystalline polymorphs, all of which are envisaged. The structure may alternatively be of the enzyme in free form or in the form of some other complex such as with Mn, or with other Fe or ACV analogues, or enzyme inhibitors, or other enzyme modifiers. Preferably the second enzyme is the same as the first enzyme e.g. the 3D structure of IPNS is used as a basis for modifying IPNS. Alternatively the 3D structure of one first enzyme may be used as a basis for modifying a second structurally related enzyme.

Central to the elucidation of the structure of crystalline proteins is the discovery of conditions for the production of crystals with diffract X-rays to a sufficiently high resolution. Since the cofactors (e.g. Fe(II)) and substrates (e.g. ACV) of the family of enzymes to which IPNS, DAOCS, DACS, etc. belong are sensitive to modification by reaction with

dioxygen, the crystallisation of these enzymes is preferably carried out under an anaerobic atmosphere or one containing only a very low concentration of dioxygen.

The modified enzyme(s) may be used *in vitro* or introduced via recombinant molecular biology techniques into an organism so that new materials can be fermented. It is recognised that multiple modifications may have to be made to an enzyme in order to change its substrate/product selectivity, and/or improve it efficiency. It is recognised that more than one modified enzyme may be used to effect the desired transformation. It is recognised that in order to change the nature of the enzyme-substrate/intermediate/product interactions at a particular enzyme-substrate/intermediate interface modifications may be made to the enzyme either immediately at the interface or away from it. It is recognised that the modifications may result in hybrid enzymes containing sequences from, e.g. IPNS and DAOCS or IPNS and DACS or any combination of IPNS, DAOCS, DACS or DAOCS/DACS or other related enzymes. It is also recognised that it may be desirable to further modify the organism in which the modified enzyme is to be introduced, e.g. by blocking a particular pathway in that organism (using the techniques of molecular biology) in order to modify flux through the desired/modified pathway, by introducing other enzyme activities, or by other modifications. The organism into which the modified enzyme will be used may or may not contain parts of the penicillin and cephalosporin biosynthetic machinery. The organism may already have been modified to optimise or minimise production of particular products or consumption of particular nutrients. More than one modified enzyme may be used in conjunction either *in vitro* or *in vivo* in an organism for the production of desirable products.

While modifications for numerous specific purposes are discussed below, it is possible to say in general that useful modifications will be of three kinds:

- Those which permit the enzyme to accept unnatural substrates [i.e. substrates not normally present in the organism (which may or may not be an organism in which the enzyme is naturally occurring) in which the enzyme is operating] for the preparation of new or commercially valuable anti-bacterial materials or intermediates for the production of pharmaceutical products;
- Those which enable the enzyme to produce unnatural products [i.e. products not naturally produced in the organism in which the enzyme is operating, including 3-exomethylene cephams and cephalosporins with hydrophobic side chains at the C-7 position such as phenylacetamido or phenoxyacetamido, or other unnatural side chains such as adipoyl] or improve the production of natural products of commercial value.
- Those which enhance the ability of the enzyme to produce useful products. For example DAOCS is known to catalyse the production of phenylacetylcephalosporin C from penicillin G (Baldwin *et al.*, Proceedings of the 7th International Symposium on the genetics of Industrial Micro-organisms, Abstract, p262, 1994). However, this conversion is much less efficient than the DAOCS catalysed conversion of penicillin N to DAOC. Modifications made to DAOCS may increase the efficiency of its catalytic conversion to penicillin G.

In another aspect this invention provides modified enzymes that result from application of the aforementioned techniques. These are enzymes having significant (as defined below) sequence and thus structural similarity with IPNS. Thus, structures of these enzymes may be predicted on the basis of the IPNS structures. Preferably there will be sequence similarity/identity between most of the modified enzyme and a major part of IPNS. Previous sequence comparisons (Roach *et al.*, Nature, 1995, 375, 700), using pairwise comparisons of the sequences followed by single linkage cluster analysis show that IPNS, DAOCS, DACS and

DAOC/DACS cluster with standard deviations scores of >5.0 (Barton and Sternberg, J. Mol. Biol., 1987, **198**, 327). Scores over 5.0 and preferably over 6.0 indicate that the sequence alignments will be correct within all or most of the protein secondary structural elements (Barton, Methods in Enzymol., 1990, **183**, 403); thus they have significantly similar sequences and hence structures. Note there are other criteria which may be used to ascertain significant sequence similarity for example % identity or % similarity of amino acids possessing side chains with similar physico-chemical properties (Barton and Sternberg, J. Mol. Biol., 1987, **198**, 327). Thus, on the basis of sequence comparisons it is possible to predict the structure of one enzyme (e.g. DAOCS, DACS or DAOC/DACS) from another (e.g. IPNS). Further, it is recognised that although two enzymes may have structures in which secondary structural elements are largely or wholly conserved, differences in the structures of the two enzymes may result from the side chains of the amino acids forming the secondary structural elements. These differences, which may alter the substrate/product selectivities of the compared enzymes, may be predictable if the three dimensional structure of one of the enzymes is known. An example: the natural substrate for IPNS, ACV, has an L-configured aminoadipoyl side chain, whereas the substrates for DAOCS, DACS and DAOC/DACS, i.e. penicillin N and DAOC, have D-configured aminoadipoyl side chains. This difference in selectivity may result from the different arrangement of amino acid side chain binding sites between IPNS and DAOCS, DACS, and DAOC/DACS, Further, it is recognised that there may be significant variations between enzymes which show significant sequence/structural similarity (i.e. with standard deviation scores >5.0) in exterior regions of the enzymes, e.g. in loops and at the N- and C- termini. The relative importance of these regions in substrate binding may be predicted by comparison with a known crystal structure of an enzyme with significant sequence similarity.

In one aspect, at least one of the following amino acid residues is modified:

R287; R87; R88; Y189; S183; Y91; F285; Q330; T331; V185; L106; C104; V217; L324; L317; I325; L321; S210.

The residue numbering herein is taken from the paper Nature, 1995, 375, 700-704 referred to above. These modifications are expected to have an effect on side chain substituents at the 6-position of the penicillin molecule, or the 7-position of the cephalosporin molecule. In each case, the stated amino acid residue may be replaced by the residue of any other amino acid. But in order to change the selectivity of the enzyme to accept substrates with hydrophilic or neutral side chains, the replacement is preferably to make the side chain binding pocket more hydrophobic.

In another aspect at least one of the following amino acid residues is modified:

V272; L231; L223; P283; T221; F211; F285; Q330; I187; V185; Y189; R279; S281; N230; Q225; N252; S210.

These modifications are expected to be associated with changes in the ring structure of the penicillin/cephalosporin molecule.

There follow examples of specific changes envisaged as a result of these modifications.

a) The structure of IPNS is modified in its active site region to accept unnatural substrates to produce penicillins or other bicyclic β-lactams of commercial use with hydrophobic side chains (Scheme 5). The process may include the following modifications (other modifications based on the use of the crystal structure of IPNS are not excluded):

Note, R87F/A/G/V/L/I/T/W/M/C/N/Q/P/S/T/E/D/R/K/H indicates that residue arginine-87, using the *Aspergillus nidulans* IPNS numbering scheme is modified to phenylalanine or alanine etc. See Roach *et al* Nature, 1995, 375, 700-704.).

R287F/A/G/V/L/I/W/M/C/N/Q/P/S/E/D/K/H/Y
R87F/A/G/V/L/I/W/M/C/N/Q/P/S/E/D/K/H/Y
Y189F/A/G/V/L/I/W/M/C/N/Q/P/S/E/D/K/H/R
S183F/A/G/V/L/I/W/M/C/N/Q/P/T/E/D/K/H/R/Y
Y91F/A/G/V/L/I/W/M/C/N/Q/P/S/T/E/D/K/H/R
F285A/G/V/L/I/W/M/C/N/Q/P/S/T/E/D/R/K/H/Y
Q330F/A/G/V/L/I/W/M/C/N/P/S/T/E/D/R/K/H/Y
T331F/A/G/V/L/I/W/M/C/N/P/S/E/D/R/K/H/Q/Y
V185F/A/G/L/I/W/T/M/C/N/P/S/E/D/R/K/H/Q/Y
L106F/A/G/V/I/T/W/M/C/N/P/S/E/D/R/K/H/Q/Y
C104F/A/G/V/L/I/T/W/M/N/P/S/E/D/R/K/H/Q/Y
V217F/A/G/L/I/T/W/M/C/N/P/S/E/D/R/K/H/Q/Y
L324F/A/G/V/I/T/W/M/C/N/P/S/E/D/R/K/H/Q/Y
L317F/A/G/V/I/T/W/M/C/N/P/S/E/D/R/K/H/Q/Y
I325F/A/G/V/L/T/W/M/C/N/P/S/E/D/R/K/H/Q/Y
L321F/A/G/V/I/T/W/M/C/N/P/S/E/D/R/K/H/Q/Y
S210F/A/G/V/I/L/T/W/M/C/N/P/E/D/R/K/H/Q/Y

Note in these and in subsequently proposed modifications the amino acid residue numbering scheme is based upon that used for *A. nidulans* IPNS and the sequence alignments in Roach *et al* Nature, 1995, 375, 700-704, e.g. arginine-87 in IPNS remains named as arginine-87 for other aligned enzymes.

It is recognised that modifications to the side chain binding interactions and the valinyl binding interactions of IPNS may have to be made in conjunction with each other or with other modifications in order to produce a useful catalyst with the desired properties. Other modifications based on the use of the three dimensional structures of IPNS, DACS, DAOCS, DAOCS/DACS, other sequence related enzymes or complexes of these enzymes to their substrates, intermediates, modifiers, products or

inhibitors are not excluded.

b) The structure of IPNS is modified in its active site region to accept natural or unnatural substrates to produce bicyclic β-lactams other than penicillins of commercial use (Scheme 6). For example the region of IPNS interacting with the valinyl residue of ACV may be modified such that IPNS produces 3-exomethylenecephams from ACV or other substrates for IPNS. The process may include the following modifications.

V272F/A/G/I/L/W/M/C/N/P/S/T/E/D/R/K/H/Q/Y
L231F/A/G/V/I/W/M/C/N/P/S/T/E/D/R/K/H/Q/Y
L223F/A/G/V/I/W/M/C/N/P/S/T/E/D/R/K/H/Q/Y
P283F/A/G/V/I/L/W/M/C/N/S/T/E/D/R/K/H/Q/Y
T221F/A/G/V/I/L/W/M/C/N/P/S/E/D/R/K/H/Q/Y
F211A/G/V/I/L/W/M/C/N/P/S/T/E/D/R/K/H/Q/Y
F285A/G/V/I/L/W/M/C/N/P/S/T/E/D/R/K/H/Q/Y
Q330F/A/G/V/I/L/W/M/C/N/P/S/T/E/D/R/K/H/Y
I187F/A/G/L/W/T/M/C/N/P/S/T/E/D/R/K/H/Q/Y
V185F/A/G/I/L/W/M/C/N/P/S/T/E/D/R/K/H/Q/Y
Y189F/A/G/V/I/L/W/M/C/N/P/S/T/E/D/R/K/H/Q
R279F/A/G/V/I/L/W/M/C/N/P/S/T/E/D/K/H/Q/Y
S281F/A/G/V/I/L/W/M/C/N/P/T/E/D/R/K/H/Q/Y
N230F/A/G/V/I/L/W/M/C/P/S/T/E/D/R/K/H/Q/Y
Q225F/A/G/V/I/L/W/M/C/N/P/S/T/E/D/R/K/H/Y
N252F/A/G/V/I/L/W/M/C/P/S/T/E/D/R/K/H/Q/Y
S210F/A/G/V/I/L/T/W/M/C/N/P/E/D/R/K/H/Q/Y

It is recognised that modifications may have to be made in conjunction with each other or with other modifications to IPNS in order to produce a useful catalyst with the desired properties. Other modifications

based on the use of the three dimensional structure of IPNS, DACS, DAOCS, DAOCS/DACS, other sequence related enzymes or complexes of these enzymes to their substrates, intermediates, modifiers, products or inhibitors are not excluded.

c) The side chain binding interactions of IPNS are modified such that 6-aminopenicillins or other bicylic β-lactams may be produced *in vitro* or *in vivo* from dipeptides, such as cysteinyl-valine or other dipeptides (Scheme 7). Dipeptides may be produced (either *in vitro* or *in vivo)* by the use of a peptide synthetase enzyme, such as ACV synthetase (which may be modified by mutagenesis or other techniques to optimise dipeptide production) or by chemical synthesis. The process may include the following modifications:

R287F/A/G/V/L/I/W/M/C/N/Q/P/S/T/E/D/K/H/Y
R87F/A/G/V/L/I/W/M/C/N/Q/P/S/T/E/D/K/H/Y
Y189F/A/G/V/L/I/W/M/C/N/Q/P/S/T/E/D/K/H/R
S183F/A/G/V/L/I/W/M/C/N/Q/P/T/E/D/K/H/R/Y
Y91F/A/G/V/L/I/W/M/C/N/Q/P/S/T/E/D/K/H/R
F285A/G/V/L/I/W/M/C/N/Q/P/S/T/E/D/R/K/H/Y
Q330F/A/G/V/L/I/W/M/C/N/P/S/T/E/D/R/K/H/Y
T331F/A/G/V/L/I/W/M/C/N/P/S/E/D/R/K/H/Q/Y
V185F/A/G/L/I/W/M/C/N/P/S/T/E/D/R/K/H/Q/Y
L106F/A/G/V/I/W/M/C/N/P/S/T/E/D/R/K/H/Q/Y
C104F/A/G/V/L/I/W/M/N/P/S/T/E/D/R/K/H/Q/Y
V217F/A/G/L/I/W/M/C/N/P/S/T/E/D/R/K/H/Q/Y
L324F/A/G/V/I/W/M/C/N/P/S/T/E/D/R/K/H/Q/Y
L317F/A/G/V/I/W/M/C/N/P/S/T/E/D/R/K/H/Q/Y
I325F/A/G/V/L/W/M/C/N/P/S/T/E/D/R/K/H/Q/Y
L321F/A/G/V/I/W/M/C/N/P/S/T/E/D/R/K/H/Q/Y

S210F/A/G/V/I/L/T/W/M/C/N/P/E/D/R/K/H/Q/Y

It is recognised that these modifications may have to be made in conjunction with each other or with other modifications in order to produce a useful catalyst with the desired properties. Other modifications based on the use of the three dimensional structure of IPNS, DACS, DAOCS, DAOCS/DACS, other sequence related enzymes or complexes of these enzymes to their substrates, intermediates, modifiers, products or inhibitors are not excluded.

d) The side chain binding interactions of IPNS are modified such that penams without any substituent at the 6-position or other bicylic β-lactams, without any substituent at the 6-position, may be produced *in vitro* or *in vivo* from dipeptides or amide substrates, such as 3-mercaptopropionyl-valine or other dipeptides or amides (Scheme 8). The dipeptides or amides may be produced (either in vitro or in vivo) by the use of a peptide synthetase enzyme, such as ACV synthetase (which may be modified by mutagenesis or other techniques to optimise dipeptide production) or by chemical synthesis. The process may include the following modifications:

R287F/A/G/V/L/I/W/M/C/N/Q/P/S/T/E/D/K/H/Y
R87F/A/G/V/L/I/W/M/C/N/Q/P/S/T/E/D/K/H/Y
Y189F/A/G/V/L/I/W/M/C/N/Q/P/S/T/E/D/K/H/R
S183F/A/G/V/L/I/W/M/C/N/Q/P/T/E/D/K/H/R/Y
Y91F/A/G/V/L/I/W/M/C/N/Q/P/S/T/E/D/K/H/R
F285A/G/V/L/I/W/M/C/N/Q/P/S/T/E/D/R/K/H/Y
Q330F/A/G/V/L/I/W/M/C/N/P/S/T/E/D/R/K/H/Y
T331F/A/G/V/L/I/W/M/C/N/P/S/E/D/R/K/H/Q/Y
V185F/A/G/L/I/W/M/C/N/P/S/T/E/D/R/K/H/Q/Y

L106F/A/G/V/I/W/M/C/N/P/S/T/E/D/R/K/H/Q/Y
C104F/A/G/V/L/I/W/M/N/P/S/T/E/D/R/K/H/Q/Y
V217F/A/G/L/I/W/M/C/N/P/S/T/E/D/R/K/H/Q/Y
L324F/A/G/V/I/W/M/C/N/P/S/T/E/D/R/K/H/Q/Y
L317F/A/G/V/I/W/M/C/N/P/S/T/E/D/R/K/H/Q/Y
I325F/A/G/V/L/W/M/C/N/P/S/T/E/D/R/K/H/Q/Y
L321F/A/G/V/I/W/M/C/N/P/S/T/E/D/R/K/H/Q/Y
S210F/A/G/V/I/L/T/W/M/C/N/P/E/D/R/K/H/Q/Y

It is recognised that these modifications may have to be made in conjunction with each other or with other modifications in order to produce a useful catalyst with the desired properties. Other modifications based on the use of the three dimensional structure of IPNS, DACS, DAOCS, DAOCS/DACS, other sequence related enzymes or complexes of these enzymes to their substrates, intermediates, products, modifiers, or inhibitors are not excluded.

e) IPNS is modified to produce 3-exomethylenecephams with hydrophobic or other unnatural side chains (Scheme 9) (or other intermediates for use in the preparation of cephalosporin antibiotics, e.g. Cephachlor. The process will involve modification of both the side chain binding interactions of IPNS substrates and of the valine binding interactions and may involve the use of ACV as a substrate or the use of other unnatural substrates. The process may include the following modifications, which may be made in conjunction with each other:

R287F/A/G/V/L/I/W/M/C/N/Q/P/S/T/E/D/K/H/Y
R87F/A/G/V/L/I/W/M/C/N/Q/P/S/T/E/D/K/H/Y
Y189F/A/G/V/L/I/W/M/C/N/Q/P/S/T/E/D/K/H/R
S183F/A/G/V/L/I/W/M/C/N/Q/P/T/E/D/K/H/R/Y

Y91F/A/G/V/L/I/W/M/C/N/Q/P/S/T/E/D/K/H/R
F285A/G/V/L/I/W/M/C/N/Q/P/S/T/E/D/R/K/H/Y
Q330F/A/G/V/L/I/W/M/C/N/P/S/T/E/D/R/K/H/Y
T331F/A/G/V/L/I/W/M/C/N/P/S/E/D/R/K/H/Q/Y
V185F/A/G/L/I/W/M/C/N/P/S/T/E/D/R/K/H/Q/Y
L106F/A/G/L/I/W/M/C/N/P/S/T/E/D/R/K/H/Q/Y
C104F/A/G/V/L/I/W/M/N/P/S/T/E/D/R/K/H/Q/Y
V217F/A/G/L/IW/M/C/N/P/S/T/E/D/R/K/H/Q/Y
L324F/A/G/V/I/W/M/C/N/P/S/T/E/D/R/K/H/Q/Y
L317F/A/G/V/I/W/M/C/N/P/S/T/E/D/R/K/H/Q/Y
I325F/A/G/V/L/W/M/C/N/P/S/T/E/D/R/K/H/Q/Y
L321F/A/G/V/I/W/M/C/N/P/S/T/E/D/R/K/H/Q/Y
V272F/A/G/I/L/W/M/C/N/P/S/T/E/D/R/K/H/Q/Y
L231F/A/G/V/IW/M/C/N/P/S/T/E/D/R/K/H/Q/Y
L223F/A/G/V/I/W/M/C/N/P/S/T/E/D/R/K/H/Q/Y
P283F/A/G/V/I/L/W/M/C/N/S/T/E/D/R/K/H/Q/Y
T221F/A/G/V/I/L/W/M/C/N/P/S/E/D/R/K/H/Q/Y
F211A/G/V/I/L/W/M/C/N/P/S/T/E/D/R/K/H/Q/Y
I187F/A/G/L/W/M/C/N/P/S/T/E/D/R/K/H/Q/Y/V
V185F/A/G/I/L/W/M/C/N/P/S/T/E/D/R/K/H/Q/Y
Y189F/A/G/V/I/L/W/M/C/N/P/S/T/E/D/R/K/H/Q
R279F/A/G/V/I/L/W/M/C/N/P/S/T/E/D/K/H/Q/Y
S281F/A/G/V/I/L/W/M/C/N/P/T/E/D/R/K/H/Q/Y
N230F/A/G/V/I/L/W/M/C/P/S/T/E/D/R/K/H/Q/Y
Q225F/A/G/V/I/L/W/M/C/N/P/S/T/E/D/R/K/H/Y
N252F/A/G/V/I/L/W/M/C/P/S/T/E/D/R/K/H/Q/Y
S210F/A/G/V/I/L/T/W/M/C/N/P/E/D/R/K/H/Q/Y

It is recognised that these modifications may have to be made in conjunction with each other or with other modifications in order to

produce a useful catalyst with the desired properties. Other modifications based on the use of the three dimensional structure of IPNS, DACS, DAOCS, DAOCS/DACS, other sequence related enzymes or complexes of these enzymes to their substrates, intermediates, modifiers, products or inhibitors are not excluded. The use of a modified IPNS in conjunction with another modified or unmodified oxygenase enzyme (e.g. DAOCS, DACS, DAOC/DACS) is not excluded.

f) The structure of DAOCS is modified in its active interactions region to accept substrates (*i.e.* penicillins with hydrophobic side chains, (including, but not exclusively, penicillin G and penicillin V) to produce cephalosporins or other bicyclic β-lactams of commercial use with hydrophobic or other unnatural side chains (Scheme 10). The process may include the following modifications:

R287F/A/G/V/L/I/W/M/C/N/Q/P/S/T/E/D/K/H/Y
R87F/A/G/V/L/I/W/M/C/N/Q/P/S/T/E/D/K/H/Y
R88F/A/G/V/L/I/W/M/C/N/Q/P/S/T/E/D/K/H/Y
F189R/A/G/V/L/I/W/M/C/N/Q/P/S/T/E/D/K/H/Y
C183F/A/G/V/L/I/W/M/N/Q/P/T/E/D/K/H/R/Y/S
T91F/A/G/V/L/I/W/M/C/N/Q/P/S/E/D/K/H/R/Y
F285A/G/V/L/I/W/M/C/N/Q/P/S/T/E/D/R/K/H/Y
A330F/G/V/L/I/W/M/C/N/P/S/T/E/D/R/K/H/Y/Q
P185F/A/G/L/I/W/M/C/N/V/S/T/E/D/R/K/H/Q/Y
T104F/A/G/V/L/I/T/W/M/N/P/S/E/D/R/K/H/Q/Y
M217F/A/G/L/I/T/W/C/N/P/S/E/D/R/K/H/Q/Y/V
I324F/A/G/V/T/W/M/C/N/P/S/E/D/R/K/H/Q/Y/L
I317F/A/G/V/L/T/W/M/C/N/P/S/E/D/R/K/H/Q/Y
R325F/A/G/V/L/T/W/M/C/N/P/S/E/D/K/H/Q/Y/I
Y321F/A/G/V/I/T/W/M/C/N/P/S/E/D/K/H/Q/R/L

R210F/A/G/V/I/L/T/W/M/C/N/P/E/D/R/K/H/Q/Y/S
R190F/A/G/V/I/L/T/W/M/C/N/P/E/D/R/K/H/Q/Y/S

It is recognised that these modifications may have to be made in conjunction with each other or with other modifications in order to produce a useful catalyst with the desired properties. Other modifications based on the use of the three dimensional structure of IPNS, DACS, DAOCS, DAOCS/DACS, other sequence related enzymes or complexes of these enzymes to their substrates, intermediates, modifiers, products or inhibitors are not excluded.

g) The structure of DAOCS is modified in its active interactions region to accept natural or unnatural substrates (including, but not exclusively, penicillin N, isopenicillin N, adipoyl penicillin) to produce bicyclic β-lactams other than cephalosporins of commercial use. For example the region of DAOCS interacting with the thiazolidine ring of its natural substrate penicillin N may be modified such that the modified DAOCS produces 3-exomethylenecephams from penicillin N, penicillin G, or penicillin V, or other substrates for DAOCS (Scheme 11). The process may include the following modifications:

V272F/A/G/I/L/W/M/C/N/P/S/T/E/D/R/K/H/Q/Y
L231F/A/G/V/I/W/M/C/N/P/S/T/E/D/R/K/H/Q/Y
L223F/A/G/V/I/W/M/C/N/P/S/T/E/D/R/K/H/Q/Y
V283F/A/G/I/L/W/M/C/N/S/T/E/D/R/K/H/Q/Y/P
T221F/A/G/V/I/L/W/M/C/N/P/S/E/D/R/K/H/Q/Y
M211F/A/G/V/I/L/W/M/C/N/P/S/T/E/D/R/K/H/Q/Y
L187F/A/G/I/W/M/C/N/P/S/T/E/D/R/K/H/Q/Y/V
P185F/A/G/I/L/W/M/C/N/S/T/E/D/R/K/H/Q/Y/V
F189A/G/V/I/L/W/M/C/N/P/S/T/E/D/R/K/H/Q/Y

R279F/A/G/V/I/L/W/M/C/N/P/S/T/E/D/K/H/Q/Y
S281F/A/G/V/I/L/W/M/C/N/P/T/E/D/R/K/H/Q/Y
N230F/A/G/V/I/L/W/M/C/P/S/T/E/D/R/K/H/Q/Y
Q225F/A/G/V/I/L/W/M/C/N/P/S/T/E/D/R/K/H/Y
F252F/A/G/V/I/L/W/M/C/P/S/T/E/D/R/K/H/Q/Y
R210F/A/G/V/I/L/T/W/M/C/N/P/E/D/R/K/H/Q/Y/S
R190F/A/G/V/I/L/T/W/M/C/N/P/E/D/R/K/H/Q/Y/S

It is recognised that these modifications may have to be made in conjunction with each other or with other modifications to DAOCS in order to produce a useful catalyst with the desired properties. Other modifications based on the use of the three dimensional structure of IPNS, DACS, DAOCS, DAOCS/DACS, other sequence related enzymes or complexes of these enzymes to their substrates, intermediates, modifiers, products or inhibitors are not excluded.

h) The side chain binding interactions of DAOCS are modified such that 6-aminopenicillins or other bicylic β-lactams may be produced *in vitro* or *in vivo* from 6-amino penicillins, such as 6-aminopenicillanic acid (Scheme 12). The process may include the following modifications (other modifications based on the use of the three dimensional structures of IPNS or DAOCS or DAOCS/DACS are not excluded):

R287F/A/G/V/L/I/W/M/C/N/Q/P/S/T/E/D/K/H/Y
R87F/A/G/V/L/I/W/M/C/N/Q/P/S/T/E/D/K/H/Y
R88F/A/G/V/L/I/W/M/C/N/Q/P/S/T/E/D/K/H/Y
F189R/A/G/V/L/I/W/M/C/N/Q/P/S/T/E/D/K/H/Y
C183F/A/G/V/L/I/W/M/N/Q/P/T/E/D/K/H/R/Y/S
T91F/A/G/V/L/I/W/M/C/N/Q/P/S/E/D/K/H/R/Y
F285A/G/V/L/I/W/M/C/N/Q/P/S/T/E/D/R/K/H/Y

A330F/G/V/L/I/W/M/C/N/P/S/T/E/D/R/K/H/Y/Q
P185F/A/G/L/V/I/W/M/C/N/V/S/T/E/D/R/K/H/Q/Y
T104F/A/G/V/L/I/W/M/C/N/P/S/E/D/R/K/H/Q/Y
M217F/A/G/L/I/W/M/C/N/P/S/T/E/D/R/K/H/Q/Y
I324F/A/G/V/I/W/M/C/N/P/S/T/E/D/R/K/H/Q/Y
I317F/A/G/V/I/L/W/M/C/N/P/S/T/E/D/R/K/H/Q/Y
R325F/A/G/V/L/W/M/C/N/P/S/T/E/D/K/H/Q/Y/I
Y321F/A/G/V/I/L/W/M/C/N/P/S/T/E/D/R/K/H/Q
R210F/A/G/V/I/L/T/W/M/C/N/P/E/D/R/K/H/Q/Y/S
R190F/A/G/V/I/L/T/W/M/C/N/P/E/D/R/K/H/Q/Y/S

It is recognised that these modifications may have to be made in conjunction with each other or with other modifications in order to produce a useful catalyst with the desired properties. Other modifications based on the use of the three dimensional structure of IPNS, DACS, DAOCS, DAOCS/DACS, other sequence related enzymes or complexes of these enzymes to their substrates, intermediates, modifiers, products or inhibitors are not excluded.

i) The side chain binding interactions of DAOCS is modified such that cephams or cephalosporins without any substituent at the 7-position or other bicylic β-lactams, without any substituent at the 7-position, may be produced *in vitro* or *in vivo* from penicillins or cepham substrates (Scheme 13). The penicillanic acid may be produced whether in vitro or in vivo. The process may include the following modifications:

R287F/A/G/V/L/I/W/M/C/N/Q/P/S/T/E/D/K/H/Y
R87F/A/G/V/L/I/W/M/C/N/Q/P/S/T/E/D/K/H/Y
R88F/A/G/V/L/I/W/M/C/N/Q/P/S/T/E/D/K/H/Y
F189R/A/G/V/L/I/W/M/C/N/Q/P/S/T/E/D/K/H/Y

C183F/A/G/V/L/I/W/M/N/Q/P/T/E/D/K/H/R/Y/S
T91F/A/G/V/L/I/W/M/C/N/Q/P/S/E/D/K/H/R/Y
F285A/G/V/L/I/W/M/C/N/Q/P/S/T/E/D/R/K/H/Y
A330F/G/V/L/I/W/M/C/N/P/S/T/E/D/R/K/H/Y/Q
P185F/A/G/L/I/W/M/C/N/V/S/T/E/D/R/K/H/Q/Y
T104F/A/G/V/L/I/W/M/N/C/P/S/E/D/R/K/H/Q/Y
M217F/A/G/L/I/V/W/C/N/P/S/T/E/D/R/K/H/Q/Y
I324F/A/G/V/L/W/M/C/N/P/S/T/E/D/R/K/H/Q/Y
I317F/A/G/V/L/W/M/C/N/P/S/T/E/D/R/K/H/Q/Y
R325F/A/G/V/L/W/M/C/N/P/S/T/E/D/K/H/Q/Y/I
Y321F/A/G/V/I/L/W/M/C/N/P/S/T/E/D/R/K/H/Q
R210F/A/G/V/I/L/T/W/M/C/N/P/E/D/R/K/H/Q/Y/S
R190F/A/G/V/I/L/T/W/M/C/N/P/E/D/R/K/H/Q/Y/S

It is recognised that the modifications may have to be made in conjunction with each other or with other modifications in order to produce a useful catalyst with the desired properties. Other modifications based on the use of the three dimensional structure of IPNS, DACS, DAOCS, DAOCS/DACS, other sequence related enzymes or complexes of these enzymes to their substrates, intermediates, modifiers, products or inhibitors are not excluded.

j) DAOCS is modified to produce 3-exomethylenecephams with hydrophobic side chains (Scheme 14) (or other intermediates for use in the preparation of cephalosporin antibiotics, e.g. Cefachlor.) The process will involve modification of both the side chain binding interactions of DAOCS substrates and of the thiaxolidine binding interactions and may involve the use of penicillins with hydrophobic side chains (e.g. penicillin G or V) as substrates or the use of other unnatural substrates. The process may include the following modifications (other modifications based on the use of

the three dimensional structures of IPNS or DAOCS or DAOCS/DACS are not excluded):

V272F/A/G/I/L/W/M/C/N/P/S/T/E/D/R/K/H/Q/Y
L231F/A/G/V/I/W/M/C/N/P/S/T/E/D/R/K/H/Q/Y
L223F/A/G/V/I/W/M/C/N/P/S/T/E/D/R/K/H/Q/Y
V283F/A/G/I/L/W/M/C/N/S/T/E/D/R/K/H/Q/Y/P
T221F/A/G/V/I/L/W/M/C/N/P/S/E/D/R/K/H/Q/Y
M211A/G/V/I/L/W/C/N/P/S/T/E/D/R/K/H/Q/Y/F
L187F/A/G/I/W/M/C/N/P/S/T/E/D/R/K/H/Q/Y/V
P185F/A/G/I/L/W/M/C/N/S/T/E/D/R/K/H/Q/Y/V
F189A/G/V/I/L/W/M/C/N/P/S/T/E/D/R/K/H/Q/Y
R279F/A/G/V/I/L/W/M/C/N/P/S/T/E/D/K/H/Q/Y
S281F/A/G/V/I/L/W/M/C/N/P/T/E/D/R/K/H/Q/Y
N230F/A/G/V/I/L/W/M/C/P/S/T/E/D/R/K/H/Q/Y
Q225F/A/G/V/I/L/W/M/C/N/P/S/T/E/D/R/K/H/Y
F252A/G/V/I/L/W/M/C/N/P/S/T/E/D/R/K/H/Q/Y
R287F/A/G/V/L/I/W/M/C/N/Q/P/S/T/E/D/K/H/Y
R87F/A/G/V/L/I/W/M/C/N/Q/P/S/T/E/D/K/H/Y
R88F/A/G/V/L/I/W/M/C/N/Q/P/S/T/E/D/K/H/Y
C183F/A/G/V/L/I/W/M/N/Q/P/T/E/D/K/H/R/Y/S
T91F/A/G/V/L/I/W/M/C/N/Q/P/S/E/D/K/H/R/Y
F285A/G/V/L/I/W/M/C/N/Q/P/S/T/E/D/R/K/H/Y
A330F/G/V/L/I/W/M/C/N/P/S/T/E/D/R/K/H/Y/Q
P185F/A/G/L/I/W/M/C/N/V/S/T/E/D/R/K/H/Q/Y
T104F/A/G/V/L/I/W/M/N/P/S/T/E/D/R/K/H/Q/Y
M217F/A/G/L/I/V/W/C/N/P/S/T/E/D/R/K/H/Q/Y
I324F/A/G/L/V/W/M/C/N/P/S/T/E/D/R/K/H/Q/Y
I317F/A/G/V/L/W/M/C/N/P/S/T/E/D/R/K/H/Q/Y
R325F/A/G/V/L/W/M/C/N/P/S/T/E/D/K/H/Q/Y/I

Y321F/A/G/V/I/W/M/C/N/P/S/T/E/D/R/K/H/Q/L
R210F/A/G/V/I/L/T/W/M/C/N/P/E/D/R/K/H/Q/Y/S
R190F/A/G/V/I/L/T/W/M/C/N/P/E/D/R/K/H/Q/Y/S

It is recognised that these modifications may have to be made in conjunction with each other or with other modifications in order to produce a useful catalyst with the desired properties. Other modifications based on the use of the three dimensional structure of IPNS, DACS, DAOCS, DAOCS/DACS, other sequence related enzymes or complexes of these enzymes to their substrates, intermediates, modifiers, products or inhibitors are not excluded.

k) The structure of DACS is modified in its active site region to accept substrates with hydrophobic side chains, including, but not exclusively, penicillin N, penicillin G and penicillin V) to produce cephalosporins or other bicyclic β-lactams of commercial use with hydrophobic or other unnatural side chains (Scheme 15) . The process may include the following modifications:

R287F/A/G/V/L/I/W/M/C/N/Q/P/S/T/E/D/K/H/Y
R87F/A/G/V/L/I/W/M/C/N/Q/P/S/T/E/D/K/H/Y
R88F/A/G/V/L/I/W/M/C/N/Q/P/S/T/E/D/K/H/Y
F189R/A/G/V/L/I/W/M/C/N/Q/P/S/T/E/D/K/H/Y
C183F/A/G/V/L/I/W/M/N/Q/P/T/E/D/K/H/R/Y/S
S91F/A/G/V/L/I/W/M/C/N/Q/P/T/E/D/K/H/R/Y
F285A/G/V/L/I/W/M/C/N/Q/P/S/T/E/D/R/K/H/Y
A330F/G/V/L/I/W/M/C/N/P/S/T/E/D/R/K/H/Y/Q
P185F/A/G/L/I/W/M/C/N/V/S/T/E/D/R/K/H/Q/Y
T104F/A/G/V/L/I/W/M/N/P/S/E/D/R/K/H/Q/Y/C
L317F/A/G/V/I/W/M/C/N/P/S/T/E/D/R/K/H/Q/Y

R325F/A/G/V/L/W/M/C/N/P/S/T/E/D/K/H/Q/Y/I
Y321F/A/G/V/I/W/M/C/N/P/S/T/E/D/R/K/H/Q/L
R210F/A/G/V/I/L/T/W/M/C/N/P/E/D/R/K/H/Q/Y/S
R190F/A/G/V/I/L/T/W/M/C/N/P/E/D/R/K/H/Q/Y/S

It is recognised that these modifications may have to be made in conjunction with each other or with other modifications in order to produce a useful catalyst with the desired properties. Other modifications based on the use of the three dimensional structure of IPNS, DACS, DAOCS, DAOCS/DACS, other sequence related enzymes or complexes of these enzymes to their substrates, intermediates, modifiers, products or inhibitors are not excluded.

l) The structure of DACS is modified in its active site region to accept natural or unnatural substrates (including, but not exclusively, penicillin N, adipoyl penicillin) to produce bicyclic β-lactams other than cephalosporins of commercial use (Scheme 16). For example the region of DAOCS interacting with the thiazolidine ring of its natural substrate penicillin N may be modified such that the modified DAOCS produces 3-exomethylenecephams from penicillin N, penicillin G, or penicillin V, or other substrates for DAOCS. The process may include the following modifications

V272F/A/G/I/L/W/M/C/N/P/S/T/E/D/R/K/H/Q/Y
L231F/A/G/V/I/W/M/C/N/P/S/T/E/D/R/K/H/Q/Y
L223F/A/G/V/I/W/M/C/N/P/S/T/E/D/R/K/H/Q/Y
V283F/A/G/I/L/W/M/C/N/S/T/E/D/R/K/H/Q/Y/P
T221F/A/G/V/I/L/W/M/C/N/P/S/E/D/R/K/H/Q/Y
M211A/G/V/I/L/W/C/N/P/S/T/E/D/R/K/H/Q/Y/F
L187F/A/G/I/W/M/C/N/P/S/T/E/D/R/K/H/Q/Y/V

P185F/A/G/I/L/W/M/C/N/S/T/E/D/R/K/H/Q/Y/V
R279F/A/G/V/I/L/W/M/C/N/P/S/T/E/D/K/H/Q/Y
S281F/A/G/V/I/L/W/M/N/C/N/P/T/E/D/R/K/H/Q/Y
N230F/A/G/V/I/L/W/M/C/P/S/T/E/D/R/K/H/Q/Y
Q225F/A/G/V/I/L/W/M/N/C/N/P/S/T/E/D/R/K/H/Y
F252F/A/G/V/I/L/W/M/N/C/P/S/T/E/D/R/K/H/Q/Y
R210F/A/G/V/I/L/T/W/M/C/N/P/E/D/R/K/H/Q/Y/S

It is recognised that these modifications may have to be made in conjunction with each other or with other modifications in order to produce a useful catalyst with the desired properties. Other modifications based on the use of the three dimensional structure of IPNS, DACS, DAOCS, DAOCS/DACS, other sequence related enzymes or complexes of these enzymes to their substrates, intermediates, modifiers, products or inhibitors are not excluded.

m) The side chain binding interactions of DACS are modified such that 7-aminocephems or 7-aminocephams (including 3-exomethylencephams) or other bicylic β-lactams may be produced *in vitro* or *in vivo* from 6-amino penicillins (such as 6-aminopenicillanic acid) or cephams or cephems (Scheme 17). The process may include the following modifications:

R287F/A/G/V/L/I/W/M/C/N/Q/P/S/T/E/D/K/H/Y
R87F/A/G/V/L/I/W/M/C/N/Q/P/S/T/E/D/K/H/Y
R88F/A/G/V/L/I/W/M/C/N/Q/P/S/T/E/D/K/H/Y
F189R/A/G/V/L/I/W/M/C/N/Q/P/S/T/E/D/K/H/Y
C183F/A/G/V/L/I/W/M/N/Q/P/T/E/D/K/H/R/Y/S
S91F/A/G/V/L/I/W/M/C/N/Q/P/T/E/D/K/H/R/Y
F285A/G/V/L/I/W/M/C/N/Q/P/S/T/E/D/R/K/H/Y

A330F/G/V/L/I/W/M/C/N/P/S/T/E/D/R/K/H/Y/Q
P185F/A/G/L/I/W/M/C/N/V/S/T/E/D/R/K/H/Q/Y
T104F/A/G/V/L/I/W/M/N/P/S/E/D/R/K/H/Q/Y/C
L317F/A/G/V/I/W/M/C/N/P/S/T/E/D/R/K/H/Q/Y.
R325F/A/G/V/L/W/M/C/N/P/S/T/E/D/K/H/Q/Y/I
Y321F/A/G/V/I/W/M/C/N/P/S/T/E/D/R/K/H/Q/L
R210F/A/G/V/I/L/T/W/M/C/N/P/E/D/R/K/H/Q/Y/S
R190F/A/G/V/I/L/T/W/M/C/N/P/E/D/R/K/H/Q/Y/S

It is recognised that these modifications may have to be made in conjunction with each other or with other modifications in order to produce a useful catalyst with the desired properties. Other modifications based on the use of the three dimensional structure of IPNS, DACS, DAOCS, DAOCS/DACS, other sequence related enzymes or complexes of these enzymes to their substrates, intermediates, modifiers, products or inhibitors are not excluded.

n) The side chain binding interactions of DACS are modified such that cephams or cephalosporins without any substituent at the 7-position or other bicylic β-lactams, without any substituent at the 7-position, may be produced *in vitro* or *in vivo* from penicillins or cepham substrates, such as penicillanic acid (Scheme 18). The penicillanic acid may be produced whether in vitro or in vivo. The process may include the following modifications:

R287F/A/G/V/L/I/W/M/C/N/Q/P/S/T/E/D/K/H/Y
R87F/A/G/V/L/I/W/M/C/N/Q/P/S/T/E/D/K/H/Y
R88F/A/G/V/L/I/W/M/C/N/Q/P/S/T/E/D/K/H/Y
F189R/A/G/V/L/I/W/M/C/N/Q/P/S/T/E/D/K/H/Y
C183F/A/G/V/L/I/W/M/N/Q/P/T/E/D/K/H/R/Y/S

S91F/A/G/V/L/I/W/M/C/N/Q/P/T/E/D/K/H/R/Y
F285A/G/V/L/I/W/M/C/N/Q/P/S/T/E/D/R/K/H/Y
A330F/G/V/L/I/W/M/C/N/P/S/T/E/D/R/K/H/Y/Q
P185F/A/G/L/I/W/M/C/N/V/S/T/E/D/R/K/H/Q/Y
T104F/A/G/V/L/I/W/M/N/P/S/E/D/R/K/H/Q/Y/C
L317F/A/G/V/I/W/M/C/N/P/S/T/E/D/R/K/H/Q/Y
R325F/A/G/V/L/W/M/C/N/P/S/T/E/D/K/H/Q/Y/I
Y321F/A/G/V/I/W/M/C/N/P/S/T/E/D/R/K/H/Q/L
R210F/A/G/V/I/L/T/W/M/C/N/P/E/D/R/K/H/Q/Y/S
R190F/A/G/V/I/L/T/W/M/C/N/P/E/D/R/K/H/Q/Y/S

It is recognised that these modifications may have to be made in conjunction with each other or with other modifications in order to produce a useful catalyst with the desired properties. Other modifications based on the use of the three dimensional structure of IPNS, DACS, DAOCS, DAOCS/DACS, other sequence related enzymes or complexes of these enzymes to their substrates, intermediates, modifiers, products or inhibitors are not excluded.

o) DACS is modified to produce 3-exomethylenecephams with hydrophobic side chains (or other intermediates for use in the preparation of cephalosporin antibiotics, e.g. Cephachlor.) (Scheme 19). The process will involve modification of both the side chain binding interactions of DACS substrates and of the thiaxolidine or cepham binding interactions and may involve the use of penicillins with hydrophobic side chains (e.g. penicillin G or V) as substrates or the use of other unnatural substrates. The process may include the following modifications:

V272F/A/G/I/L/W/M/C/N/P/S/T/E/D/R/K/H/Q/Y
L231F/A/G/V/I/W/M/C/N/P/S/T/E/D/R/K/H/Q/Y

L223F/A/G/V/I/W/M/C/N/P/S/T/E/D/R/K/H/Q/Y
V283F/A/G/I/L/W/M/C/N/S/T/E/D/R/K/H/Q/Y/P
T221F/A/G/V/I/L/W/M/C/N/P/S/E/D/R/K/H/Q/Y
M211A/G/V/I/L/W/C/N/P/S/T/E/D/R/K/H/Q/Y/F
L187F/A/G/I/W/M/C/N/P/S/T/E/D/R/K/H/Q/Y/V
P185F/A/G/I/L/W/M/C/N/S/T/E/D/R/K/H/Q/Y/V
R279F/A/G/V/I/L/W/M/C/N/P/S/T/E/D/K/H/Q/Y
S281F/A/G/V/I/L/W/M/N/C/N/P/T/E/D/R/K/H/Q/Y
N230F/A/G/V/I/L/W/M/C/P/S/T/E/D/R/K/H/Q/Y
Q225F/A/G/V/I/L/W/M/N/C/N/P/S/T/E/D/R/K/H/Y
F252F/A/G/V/I/L/W/M/N/C/P/S/T/E/D/R/K/H/Q/Y
R287F/A/G/V/L/I/W/M/C/N/Q/P/S/T/E/D/K/H/Y
R87F/A/G/V/L/I/W/M/C/N/Q/P/S/T/E/D/K/H/Y
R88F/A/G/V/L/I/W/M/C/N/Q/P/S/T/E/D/K/H/Y
F189R/A/G/V/L/I/W/M/C/N/Q/P/S/T/E/D/K/H/Y
C183F/A/G/V/L/I/W/M/N/Q/P/T/E/D/K/H/R/Y/S
S91F/A/G/V/L/I/W/M/C/N/Q/P/T/E/D/K/H/R/Y
F285A/G/V/L/I/W/M/C/N/Q/P/S/T/E/D/R/K/H/Y
A330F/G/V/L/I/W/M/C/N/P/S/T/E/D/R/K/H/Y/Q
P185F/A/G/L/I/W/M/C/N/V/S/T/E/D/R/K/H/Q/Y
T104F/A/G/V/L/I/W/M/N/P/S/E/D/R/K/H/Q/Y/C
L317F/A/G/V/I/W/M/C/N/P/S/T/E/D/R/K/H/Q/Y
R325F/A/G/V/L/W/M/C/N/P/S/T/E/D/K/H/Q/Y/I
Y321F/A/G/V/I/W/M/C/N/P/S/T/E/D/R/K/H/Q/L
R210F/A/G/V/I/L/T/W/M/C/N/P/E/D/R/K/H/Q/Y/S

It is recognised that these modifications may have to be made in conjunction with each other or with other modifications in order to produce a useful catalyst with the desired properties. Other modifications based on the use of the three dimensional structure of IPNS, DACS,

DAOCS, DAOCS/DACS, other sequence related enzymes or complexes of these enzymes to their substrates, intermediates, modifiers, products or inhibitors are not excluded.

p) The structure of DAOCS/DACS is modified in its active site region to accept natural or unnatural substrates (including, but not exclusively, penicillin N, adipoyl penicillin) to produce bicyclic β-lactams other than cephalosporins of commercial use (Scheme 20). For example the region of DAOCS/DACS interacting with the thiazolidine ring of its natural substrate penicillin N (or the cepham ring of DAOC) may be modified such that the modified DAOCS/DACS produces 3-exomethylenecephams from penicillin N, penicillin G, or penicillin V, or other substrates for DAOCS/DACS. The process may include the following modifications:

V272F/A/G/I/L/W/M/C/N/P/S/T/E/D/R/K/H/Q/Y
L231F/A/G/V/I/W/M/C/N/P/S/T/E/D/R/K/H/Q/Y
L223F/A/G/V/I/W/M/C/N/P/S/T/E/D/R/K/H/Q/Y
V283F/A/G/I/L/W/M/C/N/S/T/E/D/R/K/H/Q/Y/P
T221F/A/G/V/I/L/W/M/C/N/P/S/E/D/R/K/H/Q/Y
M211A/G/V/I/L/T/W/C/N/P/S/E/D/R/K/H/Q/Y/F
L187F/A/G/I/T/W/M/C/N/P/S/E/D/R/K/H/Q/Y/V
P185F/A/G/I/L/T/W/M/C/N/S/E/D/R/K/H/Q/Y/V
L189A/G/V/I/L/T/W/M/C/N/P/S/E/D/R/K/H/Q/Y/F
R279F/A/G/V/I/L/T/W/M/C/N/P/S/E/D/K/H/Q/Y
S281F/A/G/V/I/L/T/W/M/C/N/P/E/D/R/K/H/Q/Y
N230F/A/G/V/I/L/T/W/M/C/P/S/E/D/R/K/H/Q/Y
Q225F/A/G/V/I/L/T/W/M/C/N/P/S/E/D/R/K/H/Y
F252F/A/G/V/I/L/T/W/M/C/P/S/E/D/R/K/H/Q/Y
R210F/A/G/V/I/L/T/W/M/C/N/P/E/D/R/K/H/Q/Y/S

R190F/A/G/V/I/L/T/W/M/C/N/P/E/D/R/K/H/Q/Y/S

It is recognised that these modifications may have to be made in conjunction with each other or with other modifications in order to produce a useful catalyst with the desired properties. Other modifications based on the use of the three dimensional structure of IPNS, DACS, DAOCS, DAOCS/DACS, other sequence related enzymes or complexes of these enzymes to their substrates, intermediates, modifiers, products or inhibitors are not excluded.

q) The side chain binding interactions of DAOCS/DACS are modified such that 7-aminocephems or 7-aminocephams (including 3-exomethylencephams) or other bicylic β-lactams may be produced *in vitro* or *in vivo* from 6-amino penicillins (e.g. 6-aminopenicillanic acid) or cephams or cephems (Scheme 21). The process may include the following modifications:

R287F/A/G/V/L/I/W/M/C/N/Q/P/S/T/E/D/K/H/Y
R87F/A/G/V/L/I/W/M/C/N/Q/P/S/T/E/D/K/H/Y
R88F/A/G/V/L/I/W/M/C/N/Q/P/S/T/E/D/K/H/Y
L189F/A/G/V/L/I/W/M/C/N/Q/P/S/T/E/D/K/H/Y/R
C183F/A/G/V/L/I/W/M/N/Q/P/T/E/D/K/H/R/Y/S
S91F/A/G/V/L/I/W/M/C/N/Q/P/T/E/D/K/H/R/Y
F285A/G/V/L/I/W/M/C/N/Q/P/S/T/E/D/R/K/H/Y
A330F/G/V/L/I/W/M/C/N/P/S/T/E/D/R/K/H/Y/Q
P185F/A/G/L/I/W/M/C/N/V/S/T/E/D/R/K/H/Q/Y
T104F/A/G/V/L/I/W/M/C/N/P/S/E/D/R/K/H/Q/Y
T217F/A/G/L/I/V/W/M/C/N/P/S/E/D/R/K/H/Q/Y
M324F/A/G/V/I/L/W/C/N/P/S/T/E/D/R/K/H/Q/Y
L317F/A/G/V/I/W/M/C/N/P/S/T/E/D/R/K/H/Q/Y
R325F/A/G/V/L/W/M/C/N/P/S/T/E/D/K/H/Q/Y/I

Y321F/A/G/V/I/L/W/M/C/N/P/S/T/E/D/R/K/H/Q
R210F/A/G/V/I/L/T/W/M/C/N/P/E/D/R/K/H/Q/Y/S
R190F/A/G/V/I/L/T/W/M/C/N/P/E/D/R/K/H/Q/Y/S

It is recognised that these modifications may have to be made in conjunction with each other or with other modifications in order to produce a useful catalyst with the desired properties. Other modifications based on the use of the three dimensional structure of IPNS, DACS, DAOCS, DAOCS/DACS, other sequence related enzymes or complexes of these enzymes to their substrates, intermediates, modifiers, products or inhibitors are not excluded.

r) The side chain binding interactions of DAOCS/DACS are modified such that cephams or cephalosporins without any substituent at the 7-position or other bicylic β-lactams, without any substituent at the 7-position, may be produced *in vitro* or *in vivo* from penicillins or cepham substrates, such as penicillanic acid. The penicillanic acid may be produced whether *in vitro* or *in vivo* (Scheme 22). The process may include the following modifications:

R287F/A/G/V/L/I/W/M/C/N/Q/P/S/T/E/D/K/H/Y
R87F/A/G/V/L/I/W/M/C/N/Q/P/S/T/E/D/K/H/Y
R88F/A/G/V/L/I/W/M/C/N/Q/P/S/T/E/D/K/H/Y
L189F/A/G/V/L/I/W/M/C/N/Q/P/S/T/E/D/K/H/Y/R
C183F/A/G/V/L/I/W/M/N/Q/P/T/E/D/K/H/R/Y/S
S91F/A/G/V/L/I/W/M/C/N/Q/P/T/E/D/K/H/R/Y
F285A/G/V/L/I/W/M/C/N/Q/P/S/T/E/D/R/K/H/Y
A330F/G/V/L/I/W/M/C/N/P/S/T/E/D/R/K/H/Y/Q
P185F/A/G/L/I/W/M/C/N/V/S/T/E/D/R/K/H/Q/Y
T104F/A/G/V/L/I/W/M/C/N/P/S/E/D/R/K/H/Q/Y

T217F/A/G/L/I/V/W/M/C/N/P/S/E/D/R/K/H/Q/Y
M324F/A/G/V/I/L/W/C/N/P/S/T/E/D/R/K/H/Q/Y
L317F/A/G/V/I/W/M/C/N/P/S/T/E/D/R/K/H/Q/Y
R325F/A/G/V/L/W/M/C/N/P/S/T/E/D/K/H/Q/Y/I
Y321F/A/G/V/I/L/W/M/C/N/P/S/T/E/D/R/K/H/Q
R210F/A/G/V/I/L/T/W/M/C/N/P/E/D/R/K/H/Q/Y/S
R190F/A/G/V/I/L/T/W/M/C/N/P/E/D/R/K/H/Q/Y/S

It is recognised that these modifications may have to be made in conjunction with each other or with other modifications in order to produce a useful catalyst with the desired properties. Other modifications based on the use of the three dimensional structure of IPNS, DACS, DAOCS, DAOCS/DACS, other sequence related enzymes or complexes of these enzymes to their substrates, intermediates, modifiers, products or inhibitors are not excluded.

s) DAOCS/DACS is modified to produce 3-exomethylenecephams with hydrophobic side chains (or other intermediates for use in the preparation of cephalosporin antibiotics, e.g. Cephachlor) (Scheme 23). The process will involve modification of both the side chain binding interactions of DAOCS/DACS substrates and of the thiaxolidine or cepham binding interactions and may involve the use of penicillins with hydrophobic side chains (*e.g.* penicillin G or V) as substrates or the use of other unnatural substrates. The process may include the following modifications:

R287F/A/G/V/L/I/W/M/C/N/Q/P/S/T/E/D/K/H/Y
R87F/A/G/V/L/I/W/M/C/N/Q/P/S/T/E/D/K/H/Y
R88F/A/G/V/L/I/W/M/C/N/Q/P/S/T/E/D/K/H/Y
L189F/A/G/V/L/I/W/M/C/N/Q/P/S/T/E/D/K/H/Y/R

S91F/A/G/V/L/I/W/M/C/N/Q/P/T/E/D/K/H/R/Y
F285A/G/V/L/I/W/M/C/N/Q/P/S/T/E/D/R/K/H/Y
A330F/G/V/L/I/W/M/C/N/P/S/T/E/D/R/K/H/Y/Q
P185F/A/G/L/I/W/M/C/N/V/S/T/E/D/R/K/H/Q/Y
T104F/A/G/V/L/I/W/M/C/N/P/S/E/D/R/K/H/Q/Y
T217F/A/G/L/I/V/W/M/C/N/P/S/E/D/R/K/H/Q/Y
M324F/A/G/V/I/L/W/C/N/P/S/T/E/D/R/K/H/Q/Y
L317F/A/G/V/I/W/M/C/N/P/S/T/E/D/R/K/H/Q/Y
R325F/A/G/V/L/W/M/C/N/P/S/T/E/D/K/H/Q/Y/I
Y321F/A/G/V/I/L/W/M/C/N/P/S/T/E/D/R/K/H/Q
V272F/A/G/I/L/W/M/C/N/P/S/T/E/D/R/K/H/Q/Y
L231F/A/G/V/I/W/M/C/N/P/S/T/E/D/R/K/H/Q/Y
L223F/A/G/V/I/W/M/C/N/P/S/T/E/D/R/K/H/Q/Y
V283F/A/G/I/L/W/M/C/N/S/T/E/D/R/K/H/Q/Y/P
T221F/A/G/V/I/L/W/M/C/N/P/S/E/D/R/K/H/Q/Y
M211A/G/V/I/L/T/W/C/N/P/S/E/D/R/K/H/Q/Y/F
L187F/A/G/I/T/W/M/C/N/P/S/E/D/R/K/H/Q/Y/V
P185F/A/G/I/L/T/W/M/C/N/S/E/D/R/K/H/Q/Y/V
F189A/G/V/I/L/T/W/M/C/N/P/S/E/D/R/K/H/Q/Y
R279F/A/G/V/I/L/T/W/M/C/N/P/S/E/D/K/H/Q/Y
S281F/A/G/V/I/L/T/W/M/C/N/P/E/D/R/K/H/Q/Y
N230F/A/G/V/I/L/T/W/M/C/P/S/E/D/R/K/H/Q/Y
Q225F/A/G/V/I/L/T/W/M/C/N/P/S/E/D/R/K/H/Y
F252F/A/G/V/I/L/T/W/M/C/P/S/E/D/R/K/H/Q/Y
R210F/A/G/V/I/L/T/W/M/C/N/P/E/D/R/K/H/Q/Y/S
R190F/A/G/V/I/L/T/W/M/C/N/P/E/D/R/K/H/Q/Y/S

It is recognised that these modifications may have to be made in conjunction with each other or with other modifications in order to produce a useful catalyst with the desired properties. Other modifications

produce a useful catalyst with the desired properties. Other modifications based on the use of the three dimensional structure of IPNS, DACS, DAOCS, DAOCS/DACS, other sequence related enzymes or complexes of these enzymes to their substrates, intermediates, modifiers, products or inhibitors are not excluded.

t) The structure of DAOC/DACS is modified in its active site region to accept substrates (i.e. penicillins with hydrophobic side chains, (including, but not exclusively, penicillin N, penicillin G and penicillin V) to produce cephalosporins or other bicyclic β-lactams of commercial use with hydrophobic or other unnatural side chains (Scheme 24). The process may include the following modifications:

R287F/A/G/V/L/I/W/M/C/N/Q/P/S/T/E/D/K/H/Y
R87F/A/G/V/L/I/W/M/C/N/Q/P/S/T/E/D/K/H/Y
R88F/A/G/V/L/I/W/M/C/N/Q/P/S/T/E/D/K/H/Y
L189F/A/G/V/L/I/W/M/C/N/Q/P/S/T/E/D/K/H/Y/R
C183F/A/G/V/L/I/W/M/N/Q/P/T/E/D/K/H/R/Y/S
S91F/A/G/V/L/I/W/M/C/N/Q/P/T/E/D/K/H/R/Y
F285A/G/V/L/I/W/M/C/N/Q/P/S/T/E/D/R/K/H/Y
A330F/G/V/L/I/W/M/C/N/P/S/T/E/D/R/K/H/Y/Q
P185F/A/G/L/I/W/M/C/N/V/S/T/E/D/R/K/H/Q/Y
T104F/A/G/V/L/I/W/M/C/N/P/S/E/D/R/K/H/Q/Y
T217F/A/G/L/I/V/W/M/C/N/P/S/E/D/R/K/H/Q/Y
M324F/A/G/V/I/L/W/C/N/P/S/T/E/D/R/K/H/Q/Y
L317F/A/G/V/I/W/M/C/N/P/S/T/E/D/R/K/H/Q/Y
R325F/A/G/V/L/W/M/C/N/P/S/T/E/D/K/H/Q/Y/I
Y321F/A/G/V/I/L/W/M/C/N/P/S/T/E/D/R/K/H/Q
R210F/A/G/V/I/L/T/W/M/C/N/P/E/D/R/K/H/Q/Y/S
R190F/A/G/V/I/L/T/W/M/C/N/P/E/D/R/K/H/Q/Y/S

It is recognised that these modifications may have to be made in conjunction with each other or with other modifications in order to produce a useful catalyst with the desired properties. Other modifications based on the use of the three dimensional structure of IPNS, DACS, DAOCS, DAOCS/DACS, other sequence related enzymes or complexes of these enzymes to their substrates, intermediates, modifiers, products or inhibitors are not excluded.

Use can also be made of the 3D structure of IPNS to determine or predict the structure of other related enzymes which are not active in the penicillin or cephalosporin biosynthesis pathway. The structural information so obtained can then be used to modify the other enzyme or for designing an inhibitor for the other enzymes. Such other enzymes include flavone synthase, prolyl hydroxylase, proline hydroxylase, lysyl hydroxylase, aspartyl hydroxylase, flvanone 3β-hydroxylase, gibberellin C-20 oxidase, gibberellin 3β-hydroxylase, *para*-hyroxyphenylpyruvate dioxygenase (HPPD), 1-aminocyclopropane-1-carboxylic acid (ACC) oxidase. Specific embodiments envisaged include:

- The modification of the oxidases involved in gibberellin biosynthesis in order that modified enzymes may be introduced into plants in order to improve crop production.
- The design of inhibitors of ACC oxidase to be used for the control of fruit ripening.
- The design and use of inhibitors of prolyl hydroxylase for use in the treatment of arthritis and related diseases.

Modification of enzymes may conveniently be effected at the nucleic acid stage. Thus, the present invention envisages genes which code for the modified enzymes herein described. The nucleic acid sequence of such genes may be readily predicted. Mutations of existing wild-type genes may readily be effected e.g. by the use of commercially available mutagenesis kits.

The gene may be introduced into an expression vector by techniques which are well known. The expression vector may be used to transform a host micro-organism, such as for example *Penicillium chrysogenum* or *Acremonium chrysogenum*, again by techniques which are well known. The micro-organism should be capable of expressing the gene under fermentation conditions, e.g. by having the gene under the transcriptional and translational regulation of fungal expression signals. Such micro-organisms containing the modified gene may be used to make bicyclic β-lactams of the penicillin or cephalosporin family, again by techniques which are well known.

The following experiments were performed to demonstrate the invention.

EXAMPLE 1

A U.S.E mutagenesis kit (Phamacia) was used for all the mutagenesis reactions and a Pst I restriction site on the pET vector was selected. Selection of single and double mutants were successfully performed from colonies by restriction enzyme digestion. (Sambrook *et al*, Molecular Cloning, A Laboratory Manual, Cold Spring Harbour, USA, 1989). It was found that about 50% of colonies selected were mutants. Mutations of DAOCS (Table 1) were confirmed by sequencing according to the dideoxy method of Sanger. Mutants were designed after study of the IPNS-Mn^{2+} and the IPNS-Fe(II)-ACV structures. Polar residues with which the side chain D-α-aminoadipoyl (carboxylate and amino groups) might bind to were identified.

Almost all the mutants expressed well, except R88I, R88Q and R87Q/R287Q whereby the expression level was only about half of others. Generally the expression level of colonies was about 10~20 % of soluble protein at 27°C. Moreover, recombinant enzyme of P168V mutant was insoluble. These mutant enzymes were purified to ~60-70 % purity

with Resouce-Q column (Phamacia). The activity of each mutant with respect to penicillin N and its side-chain analogues was analysed by bioassay. It was found that R87I, R87Q, R88I and R88Q could inhibit the growth of *E coli* X580 cells using a hole-plate assay which contained penicillinase. The products of the reaction with penicillin G and wild type DAOCS also showed the same inhibition. Screening of the substrate conversion of penicillins mutants was also performed using a assay with radiolabelled α-ketoglutarate. The reaction conditions were the same as for bioassay except that [^{14}C]-α-ketoglutarate was used. The specific activities of the various mutants are summarised in Table I.

The loss of activity when using penicillin N as a substrate after mutation of arginine 287 to isoleucine or glutamine in the active site of expandase implies an important interaction of this amino acid with the carboxyl group which located in the side chain of penicillin N. This is compatible with the structural predictions for DAOCS which were suggested based on IPNS structure. On the other hand, mutation at arginine 87 to isoleucine or glutamine enhanced the activity (when using penicillin N as a substrate), whereas mutants of arginine 88 caused partial loss of activity (when using penicillin N as a substrate). Double mutations at the sites totally eliminated activity.

The specific activities of the (mutant) modified DAOCS, when using penicillin N as a substrate, support the prediction that the 3-dimensional structure of DAOCS is closely related to that of IPNS. However, not all the kinetic results can be predicted by analysis of the predicted DAOC structure, e.g. the apparent increase in activity of the R87Q modification, when using penicillin N as a substrate. Other results in Table 1 further demonstrate the invention. For example the R87Q mutant converts penicillin G to phenylacetylcephalosporin G more efficiently than the unmodified enzyme. Other results demonstrate the introduction of new activities into the modified DAOCS enzymes. For example neither oxacillin

nor piperacillin are substrates for the unmodified enzymes, but are substrates for the R87I/R287Q modified enzymes.

EXAMPLE 2

IPNS-Fe-ACV Complex

Enzyme and Substrate Preparation

Recombinant *A. nidulans* IPNS was purified as the apo-enzyme as described previously (Roach *et al*, Protein Science, 1995, **4**, 1007-1009) and stored at -80°C in 75μl aliquots (50 mg/ml in 20 mM Tris-HCl, pH 8.0). ACV (thiol form) was prepared as described previously and was further purified by HPLC [Hypersil octadecylsilane (C_{18}) column (250 x 10 mm), eluting with 10 mM NH_4CO_3, containing 4% (vol./vol.) MeOH; R_t=6.5 min at 4 ml/min], freeze dried and stored as 2 mg aliquots.

Crystallisation

Crystallisation trials were performed at 17°C under anaerobic conditions (<0.2 ppm O_2) in a glove box (Belle Technology, Portesham, Dorset, UK) using the hanging drop vapour diffusion technique. All solutions except the protein were deoxygenated by repeated evacuation followed by argon flushing (repeated three times) prior to transfer to the anaerobic glove box. Solid reagents (ACV, ferrous sulphate and sodium dithionite), all solutions except protein solutions, washed cover-slips and greased Linbro plates were left for 16 h in the glove box to further deoxygenate. IPNS solutions were transferred to the glove box immediately prior to each crystallisation experiment and mixed by repeated gentle pipetting to assist deoxygenation. To further ensure that the crystallisation experiments were done anaerobically, a coloured redox indicator was added to each well. Thus, oxidised resazurin which shows a mauve to colourless change upon dithionate reduction, was added (0.001% mass/vol.) to the stock well solutions (separate solutions, without

resazurin, were reserved for hanging drops) and sodium dithionite solution (100 mM) added dropwise until the solution in the well changed colour from mauve to colourless (Jacob, Methods in Microbiol., 1969, **2**, 91-124). Upon exposure to oxygen (either by contamination or upon withdrawing the crystallisation tray from the glove box), the solution in the well changed from colourless (reduced) to pink (partially oxidised).

A stock solution containing ferrous sulphate (5 mM), ACV (80 mM) and IPNS (50 mg/ml. 1.35 mM) was then prepared and used in random screening experiments using 6 μl drops (1:1 precipitant:protein) (Jancerik and Kim, J. Appl. Crystallog., 1991, **24**, 409). Three crystal forms were obtained using a precipitant solution containing 1.8M lithium sulphate and 100 mM Tris-HCl (pH 8.5). Crystals were not observed in analogous crystallisation experiments carried out in the absence of ACV. Crystallisation conditions were optimised by varying the protein and precipitant concentrations.

Plate crystals (Form I) typically appeared between 6 and 12 hours and reached a maximum size (typically 500 x 150 x 25 μm^3) in 48 hours. Hexagonal columnar crystals (Form II) typically appeared after 12 - 16 hours and grew to a maximum size (typically 1000 x 500 x 500 μm^3) in 1 week. The needles (Form III), with a hexagonal cross-section, appeared after *ca.* 2 weeks and were more commonly observed when using less homogenous batches of protein. In analogous experiments carried out under aerobic conditions, no crystals were observed.

Form I crystals grew spontaneously in less than half of the drops after 12 hours. After this time, Form II crystals began to grow and predominated in those drops in which plates had not grown. By using serial dilutions of microseeds prepared from either Form I or Form II crystals, it was possible to bias the growth of crystals completely to either of these morphologies. There is a delicate balance between production of the different forms since some drops contained two or all three of the

different crystal forms.

X-ray Analysis

For initial characterisation, crystals were mounted in quartz capillaries under an anaerobic atmosphere and the capillaries sealed with wax. Data were then collected (Table 4) at room temperature. Subsequently, the crystals were shown to be apparently stable to relatively short (< 1 hour) exposure to oxygen and were withdrawn from the glove box. The crystals were then rapidly transferred to a cryoprotective mother liquor (100 mM Tris-HCl pH 8.5, 20% (vol./vol.) glycerol, saturated at room temperature with lithium sulphate) and frozen using a Cryostream (Oxford Cryosystems). Data were then collected at 100 K. Data were analysed using the programs DENZO and SCALEPACK (Otinowski, Data Collection and Processing, Daresbury Laboratory, Warrington, UK (Sawyer *et al*, Eds) PL/SCI/R34, pp 55-62).

Table 4 - Crystal Statistics

Crystal Form	Diffraction Limit (nm)†	Space Group	Unit Cell Dimensions (nm)	Solvent Content (%)	Completeness (%)	Rsym (%)
I	0.11, 0.18	$P2_12_12_1$	4.68, 7.15, 10.10	38.5	95.4	5.9
II	0.21, 0.23	$P3_12_1$	10.10, 10.10, 11.567	69.5	94.0	7.2

† The first figure refers to the diffraction limit of the form I and form II crystals after respectively 30 and 10s exposures at BL19 of the European Synchrotron Radiation Facility (ESRF). The second figure refers to the diffraction limits after 30 min. exposures using a Rikagu rotating anode source operating at 60 kV and 70 mA equipped with a MAR Research

imaging plate detector. All other figures in the table refer to data collected at the ESRF. The data for form I crystals was collected using a MAR Research imaging plate detector and the data for the form II crystals on a charged coupled device detector.

Hereafter:

Table 1: The Specific activity of various DAOCS mutants analysed by the turnover of α-[^{14}C]-ketoglutarate.

Specific activity (nmol/min/mg)	Penicillin N	6-Amino-penicillanic acid (6-APA)	Adipyl-6-APA	Penicillin G	Penicillin V	Ampicillin	Carbenicillin	Ammoxicillin	Methicillin	Cloxacillin	Oxacillin	Piperacillin
Wild type	6.4±0.5*	1.0±0.2	2.7±0.4	5.1±0.4	5.3±0.3	0	0	1.4±0.6	0	1.6±0.6	0	0
R287I	0	1.7±0.6	0	0	2.3±0.2	0	0	1.1±0.04	0.2±0.1	2.7±0.6	2.0±0.09	1.8±0.2
R287Q	0	0	0	0	0	0	0	0	0	0	0	0
R87I	6.4±0.05	1.1±0.5	0	4.3±0.1	1.5±0.3	0	0	0	0	0.9±0.04	0.8±0.3	0
R87Q	13.4±0.4	0	0	7.5±0.4	3.4±0.6	0	0	0	0	0	0	0
R88I	5.3±0.8	0	0	2.5±0.5	0	0	0	0	0	0	0	0
R88Q	2.9±0.5	0	0	0.2±0.02	0	0	0	0	0	0	0	0
R87I/R287I	0	0	0	00.3±0.04	0	0	0	0	0	0	0	0
R87Q/R287I	0	0	0	0	0	0	0	0	0	0	0	0
R87I/R287Q	0	3.3±0.2	0	3.2±0.1	0.7±0.2	0	0	1.1±0.3	0	4.5±0.08	4.1±0.4	2.5±0.3
R87Q/R287Q	0	0	0	0	0	0	0	0	0	0	0	0

* Experiments were done in duplicate and values for "the penicillin uncoupled decarboxylation of α-ketoglutarate" have been subtracted.

The specific radioactivity of the α-ketoglutarate used was ca. 0.057 μCi/μmol.

N.B. "The penicillin uncoupled decarboxylation reaction" is the enzymatic turnover of α-ketoglutarate in the absence of penicillin substrate.

Table 2

CRYST1	59.200	127.000	139.600	90.00	90.00	90.00			
SCALE1		0.016892	0.000000	0.000000		0.00000			
SCALE2		0.000000	0.007874	0.000000		0.00000			
SCALE3		0.000000	0.000000	0.007163		0.00000			
ATOM	1	CB	VAL A	4	16.524	53.636	-2 826	1.00	79.63
ATOM	2	CG1	VAL A	4	15.692	54.759	-2.223	1.00	75.59
ATOM	3	CG2	VAL A	4	16.011	53.869	-2.523	1.00	77.94
ATOM	4	C	VAL A	4	14.636	52.001	-2.797	1.00	78.66
ATOM	5	O	VAL A	4	14.443	52.769	-3.987	1.00	79.44
ATOM	6	N	VAL A	4	16.880	51.117	-2.818	1.00	82.21
ATOM	7	CA	VAL A	4	16.049	52.254	-2.290	1.00	80.32
ATOM	8	N	SER A	5	13.655	52 015	-1.916	1 00	76.44
ATOM	9	CA	SER A	5	12.286	51 764	-2.350	1 00	73.85
ATOM	10	CB	SER A	5	11.583	50 804	-1.380	1 00	74.99
ATOM	11	OG	SER A	5	12 012	51 018	-0.044	1 00	76.77
ATOM	12	C	SER A	5	11 474	53 054	-2.482	1.00	70.80
ATOM	13	O	SER A	5	11.970	54 146	-2.187	1 00	70.77
ATOM	14	N	LYS A	6	10 250	52 914	-2.970	1 00	67.33
ATOM	**15**	**CA**	**LYS A**	**6**	**9 320**	**54.025**	**-3.124**	**1 00**	**64.23**
ATOM	16	CB	LYS A	6	8 403	53 799	-4.319	1.00	65.78
ATOM	17	CG	LYS A	6	8 751	54 568	-5.557	1 00	69.46
ATOM	18	CD	LYS A	6	7 579	54 445	-6.510	1 00	76.71
ATOM	19	CE	LYS A	6	7 768	55.261	-7.784	1 00	81.89
ATOM	20	NZ	LYS A	6	6 509	55 312	-8.612	1 00	83.94
ATOM	21	C	LYS A	6	8 457	54 095	-1.868	1.00	61 05
ATOM	22	O	LYS A	6	8 061	53.061	-1.325	1 00	62 18
ATOM	23	N	ALA A	7	8 166	55 304	-1.410	1.00	55.41
ATOM	24	CA	ALA A	7	7 346	55.487	-0.231	1.00	49 08
ATOM	25	CB	ALA A	7	7 632	56 853	0.393	1.00	44 79
ATOM	26	C	ALA A	7	5.875	55 363	-0.609	1.00	46.39
ATOM	27	O	ALA A	7	5 469	55 706	-1.721	1.00	44 68
ATOM	28	N	ASN A	8	5 080	54 840	0.313	1.00	45.74
ATOM	29	CA	ASN A	8	3 652	54 694	0.086	1.00	46 86
ATOM	30	CB	ASN A	8	3.041	53 759	1.142	1.00	53 92
ATOM	31	CG	ASN A	8	1.515	53 798	1.154	1.00	59.91
ATOM	32	OD1	ASN A	8	0 865	53.318	0.225	1.00	63.71
ATOM	33	ND2	ASN A	8	0 941	54 403	2.193	1.00	61.02
ATOM	34	C	ASN A	8	3 009	56.078	0.175	1.00	45.51
ATOM	35	O	ASN A	8	2 782	56.594	1.276	1.00	49.10
ATOM	36	N	VAL A	9	2 802	56.712	-0.977	1 00	42.13
ATOM	37	CA	VAL A	9	2 167	58 028	-1.026	1 00	36.18
ATOM	38	CB	VAL A	9	3.066	59 093	-1.733	1.00	31.81
ATOM	39	CG1	VAL A	9	2 425	60 459	-1.650	1.00	28.09
ATOM	40	CG2	VAL A	9	4 438	59 149	-1.100	1 00	26.59
ATOM	41	C	VAL A	9	0 835	57 869	-1.768	1 00	36 23
ATOM	42	O	VAL A	9	0.785	57 827	-3 000	1 00	39.84
ATOM	43	N	PRO A	10	-0.261	57 715	-1 018	1 00	35 13
ATOM	44	CD	PRO A	10	-0 322	57.622	0 451	1.00	33 70
ATOM	45	CA	PRO A	10	-1 588	57 549	-1 620	1 00	34 32
ATOM	46	CB	PRO A	10	-2.473	57 229	-0.422	1 00	35.22
ATOM	47	CG	PRO A	10	-1 775	57 912	0.734	1 00	34 45
ATOM	48	C	PRO A	10	-2.094	58 759	-2.390	1.00	33 02
ATOM	49	O	PRO A	10	-1.778	59 897	-2 060	1.00	36 04
ATOM	50	N	LYS A	11	-2 870	58 503	-3 434	1.00	35 45
ATOM	51	CA	LYS A	11	-3 435	59.576	-4.236	1.00	36 88
ATOM	52	CB	LYS A	11	-3 361	59.233	-5 724	1.00	31.82
ATOM	53	CG	LYS A	11	-1 958	58.944	-6.203	1 00	38.51
ATOM	54	CD	LYS A	11	-1 958	58 929	-7 722	1 00	44.67
ATOM	55	CE	LYS A	11	-0 482	58 455	-8.166	1 00	47 02
ATOM	56	NZ	LYS A	11	0 620	59 309	-7 628	1 00	53 83
ATOM	57	C	LYS A	11	-4 882	59.740	-3.798	1.00	39 16
ATOM	58	O	LYS A	11	-5.748	58 984	-4.232	1.00	46 42
ATOM	59	N	ILE A	12	-5.133	60 704	-2 917	1.00	36 94
ATOM	60	CA	ILE A	12	-6.474	60 959	-2 394	1.00	32 90
ATOM	61	CB	ILE A	12	-6.407	61 510	-0 965	1.00	25.22
ATOM	62	CG2	ILE A	12	-7.803	61 826	-0 436	1.00	19 49
ATOM	63	CG1	ILE A	12	-5.682	60.505	-0 077	1.00	26 81
ATOM	64	CD1	ILE A	12	-5.414	60.395	1.324	1.00	29 30
ATOM	65	C	ILE A	12	-7.268	61 932	-3 250	1.00	38.45
ATOM	66	O	ILE A	12	-6.729	62 919	-3.749	1.00	41.39
ATOM	67	N	ASP A	13	-8.544	61 622	-3.451	1.00	44.52
ATOM	68	CA	ASP A	13	-9.431	62.484	-4.225	1.00	46.03
ATOM	69	CB	ASP A	13	-10.555	61 684	-4.881	1.00	51.16

ATOM	70	CG	ASP A	13	-11 361	62.512	-5.869	1 00	56.62
ATOM	71	OD1	ASP A	13	-11 737	63.659	-5.544	1 00	54.34
ATOM	72	OD2	ASP A	13	-11 619	62.011	-6.984	1 00	66.60
ATOM	73	C	ASP A	13	-10 000	63.472	-3.227	1 00	44.39
ATOM	74	O	ASP A	13	-10 791	63.121	-2.354	1 00	44 73
ATOM	75	N	VAL A	14	-9 605	64.719	-3.391	1 00	44 33
ATOM	76	CA	VAL A	14	-10 003	65.785	-2.498	1 00	38 69
ATOM	77	CB	VAL A	14	-8 796	66.720	-2.338	1.00	34 66
ATOM	78	CG1	VAL A	14	-9.190	68 101	-1.875	1 00	37 77
ATOM	79	CG2	VAL A	14	-7 833	66.077	-1.365	1 00	33.42
ATOM	80	C	VAL A	14	-11.296	66 521	-2.846	1.00	39.30
ATOM	81	O	VAL A	14	-11 808	67.298	-2.036	1 00	39 59
ATOM	82	N	SER A	15	-11 891	66 202	-3.990	1.00	38.33
ATOM	83	CA	SER A	15	-13.116	66 881	-4.393	1 00	37 64
ATOM	84	CB	SER A	15	-13 686	66 298	-5.689	1.00	39.61
ATOM	85	OG	SER A	15	-14.027	64.933	-5.546	1.00	47 59
ATOM	86	C	SER A	15	-14 197	66.977	-3 324	1.00	37 35
ATOM	87	O	SER A	15	-14 691	68.066	-3 056	1.00	40.20
ATOM	88	N	PRO A	16	-14.532	65.866	-2 647	1.00	38.58
ATOM	89	CD	PRO A	16	-13 957	64 511	-2 724	1.00	40.22
ATOM	90	CA	PRO A	16	-15.574	65 918	-1.613	1.00	37.63
ATOM	91	CB	PRO A	16	-15.410	64 583	-0.901	1.00	33.25
ATOM	92	CG	PRO A	16	-14.999	63 689	-1.991	1 00	36.58
ATOM	93	C	PRO A	16	-15.439	67 066	-0.624	1.00	38.86
ATOM	94	O	PRO A	16	-16.442	67 614	-0 184	1 00	40 71
ATOM	95	N	LEU A	17	-14.200	67.444	-0.310	1.00	39.30
ATOM	96	CA	LEU A	17	-13 917	68.513	0 649	1.00	38.18
ATOM	97	CB	LEU A	17	-12 412	68.594	0.911	1.00	34.24
ATOM	98	CG	LEU A	17	-11 838	67.299	1.490	1.00	32 70
ATOM	99	CD1	LEU A	17	-10.330	67.382	1.663	1.00	27.81
ATOM	100	CD2	LEU A	17	-12 515	67.008	2 820	1.00	34.84
ATOM	101	C	LEU A	17	-14.472	69 881	0.260	1.00	41 67
ATOM	102	O	LEU A	17	-14.598	70 776	1.105	1 00	38.36
ATOM	103	N	PHE A	18	-14.774	70.043	-1.025	1.00	48.11
ATOM	104	CA	PHE A	18	-15.339	71.287	-1 551	1 00	52.21
ATOM	105	CB	PHE A	18	-14.857	71.551	-2 993	1.00	51.38
ATOM	106	CG	PHE A	18	-13.365	71.738	-3 132	1.00	49.52
ATOM	107	CD1	PHE A	18	-12.552	70.679	-3.513	1.00	50.16
ATOM	108	CD2	PHE A	18	-12.781	72.983	-2.932	1.00	47.59
ATOM	109	CE1	PHE A	18	-11.183	70.857	-3.695	1.00	50.47
ATOM	110	CE2	PHE A	18	-11.413	73 166	-3.114	1 00	44.37
ATOM	111	CZ	PHE A	18	-10.616	72 102	-3.496	1 00	45.21
ATOM	112	C	PHE A	18	-16.871	71.202	-1.550	1.00	53 42
ATOM	113	O	PHE A	18	-17.550	72.180	-1.848	1 00	53.80
ATOM	114	N	GLY A	19	-17.407	70.020	-1 259	1 00	56.82
ATOM	115	CA	GLY A	19	-18.847	69.842	-1.247	1.00	60 49
ATOM	116	C	GLY A	19	-19.502	69 931	0 120	1.00	64.67
ATOM	117	O	GLY A	19	-18.927	70 470	1.071	1.00	64.98
ATOM	118	N	ASP A	20	-20.738	69 441	0 200	1 00	69 36
ATOM	119	CA	ASP A	20	-21.507	69.443	1 449	1 00	72.36
ATOM	120	CB	ASP A	20	-22.799	70.263	1.310	1 00	76.50
ATOM	121	CG	ASP A	20	-22.543	71 760	1.234	1.00	83 77
ATOM	122	OD1	ASP A	20	-21.889	72 300	2.152	1.00	89 42
ATOM	123	OD2	ASP A	20	-23.002	72.400	0.262	1 00	85.64
ATOM	124	C	ASP A	20	-21.861	68 035	1.918	1.00	70.68
ATOM	125	O	ASP A	20	-22.433	67 865	2.992	1 00	71.00
ATOM	126	N	ASP A	21	-21.533	67 030	1.111	1 00	68.45
ATOM	127	CA	ASP A	21	-21.830	65 653	1.473	1 00	66.91
ATOM	128	CB	ASP A	21	-21.643	64.720	0.267	1 00	69.88
ATOM	129	CG	ASP A	21	-22.015	63.268	0.574	1 00	73.83
ATOM	130	OD1	ASP A	21	-22.477	62 978	1.702	1 00	76.66
ATOM	131	OD2	ASP A	21	-21.845	62 409	-0.322	1 00	76.24
ATOM	132	C	ASP A	21	-20.917	65.240	2.625	1 00	65.51
ATOM	133	O	ASP A	21	-19.785	64.800	2.419	1 00	67.20
ATOM	134	N	GLN A	22	-21.433	65.365	3.838	1 00	63.04
ATOM	135	CA	GLN A	22	-20.687	65.018	5.033	1.00	59.99
ATOM	136	CB	GLN A	22	-21.578	65.138	6.264	1.00	60.92
ATOM	137	CG	GLN A	22	-20.821	65.550	7.505	1.00	68.34
ATOM	138	CD	GLN A	22	-20.120	66.894	7.326	1.00	74.81
ATOM	139	OE1	GLN A	22	-20.632	67.793	6.649	1.00	78.00
ATOM	140	NE2	GLN A	22	-18.931	67.028	7.909	1.00	77.30
ATOM	141	C	GLN A	22	-20.104	63.623	4.971	1.00	58.00
ATOM	142	O	GLN A	22	-18.965	63.402	5.384	1.00	59.37

ATOM	143	N	ALA A	23	-20.877	62.688	4.429	1.00	55.74
ATOM	144	CA	ALA A	23	-20.448	61.294	4.323	1.00	57.85
ATOM	145	CB	ALA A	23	-21.550	60.444	3.688	1.00	57.01
ATOM	146	C	ALA A	23	-19.142	61.133	3.547	1.00	58.62
ATOM	147	O	ALA A	23	-18.180	60.534	4.040	1.00	59.15
ATOM	148	N	ALA A	24	-19.112	61.662	2.329	1.00	57.88
ATOM	149	CA	ALA A	24	-17.920	61.567	1.505	1.00	54.77
ATOM	150	CB	ALA A	24	-18.195	62.086	0.097	1.00	52.07
ATOM	151	C	ALA A	24	-16.772	62.334	2.176	1.00	52.15
ATOM	152	O	ALA A	24	-15.617	61.905	2.114	1.00	55.14
ATOM	153	N	LYS A	25	-17.097	63.443	2.835	1.00	46.23
ATOM	154	CA	LYS A	25	-16.087	64.230	3.516	1.00	42.19
ATOM	155	CB	LYS A	25	-16.690	65.505	4.112	1.00	38.59
ATOM	156	CG	LYS A	25	-16.655	66.663	3.149	1.00	33.56
ATOM	157	CD	LYS A	25	-17.022	67.980	3.806	1.00	35.21
ATOM	158	CE	LYS A	25	-18.525	68.172	3.890	1.00	37.82
ATOM	159	NZ	LYS A	25	-18.878	69.562	4.275	1.00	39.00
ATOM	160	C	LYS A	25	-15.406	63.406	4.593	1.00	43.50
ATOM	**161**	**O**	**LYS A**	**25**	**-14.186**	**63.378**	**4.688**	**1.00**	**45.05**
ATOM	162	N	MET A	26	-16.189	62.680	5.368	1.00	46.05
ATOM	163	CA	MET A	26	-15.599	61.872	6.424	1.00	51.52
ATOM	164	CB	MET A	26	-16.674	61.263	7.306	1.00	58.77
ATOM	165	CG	MET A	26	-17.065	62.138	8.503	1.00	68.62
ATOM	166	SD	MET A	26	-15.776	62.302	9.788	1.00	75.98
ATOM	167	CE	MET A	26	-15.385	60.571	10.146	1.00	72.86
ATOM	168	C	MET A	26	-14.740	60.785	5.816	1.00	49.91
ATOM	169	O	MET A	26	-13.709	60.392	6.395	1.00	49.46
ATOM	170	N	ARG A	27	-15.148	60.307	4.645	1.00	50.27
ATOM	171	CA	ARG A	27	-14.407	59.273	3.942	1.00	51.72
ATOM	172	CB	ARG A	27	-15.141	58.858	2.662	1.00	59.72
ATOM	173	CG	ARG A	27	-15.819	57.512	2.736	1.00	70.60
ATOM	174	CD	ARG A	27	-16.315	57.084	1.365	1.00	80.78
ATOM	175	NE	ARG A	27	-17.703	57.450	1.123	1.00	88.62
ATOM	176	CZ	ARG A	27	-18.115	58.133	0.056	1.00	93.71
ATOM	177	NH1	ARG A	27	-17.243	58.547	-0.867	1.00	96.83
ATOM	178	NH2	ARG A	27	-19.414	58.338	-0.135	1.00	97.09
ATOM	179	C	ARG A	27	-13.026	59.802	3.585	1.00	48.22
ATOM	180	O	ARG A	27	-12.030	59.215	3.794	1.00	49.76
ATOM	181	N	VAL A	28	-12.977	61.018	3.040	1.00	44.42
ATOM	182	CA	VAL A	28	-11.705	61.637	2.669	1.00	40.68
ATOM	183	CB	VAL A	28	-11.896	63.013	1.989	1.00	40.13
ATOM	184	CG1	VAL A	28	-10.540	63.639	1.672	1.00	40.08
ATOM	185	CG2	VAL A	28	-12.684	62.844	0.709	1.00	39.09
ATOM	186	C	VAL A	28	-10.868	62.798	3.922	1.00	41.23
ATOM	187	O	VAL A	28	-9.706	62.381	3.963	1.00	41.90
ATOM	188	N	ALA A	29	-11.510	62.271	4.981	1.00	40.14
ATOM	189	CA	ALA A	29	-10.854	62.492	6.255	1.00	39.42
ATOM	190	CB	ALA A	29	-11.873	62.936	7.274	1.00	40.42
ATOM	191	C	ALA A	29	-10.131	61.242	6.731	1.00	41.63
ATOM	192	O	ALA A	29	-8.963	61.307	7.119	1.00	42.66
ATOM	193	N	GLN A	30	-10.803	60.099	6.666	1.00	44.92
ATOM	194	CA	GLN A	30	-10.201	58.848	7.106	1.00	48.27
ATOM	195	CB	GLN A	30	-11.203	57.702	6.971	1.00	54.77
ATOM	196	CG	GLN A	30	-12.400	57.837	7.901	1.00	67.39
ATOM	197	CD	GLN A	30	-13.579	56.964	7.495	1.00	75.12
ATOM	198	OE1	GLN A	30	-13.471	56.115	6.605	1.00	77.42
ATOM	199	NE2	GLN A	30	-14.724	57.189	8.136	1.00	79.26
ATOM	200	C	GLN A	30	-8.930	58.544	6.328	1.00	47.85
ATOM	201	O	GLN A	30	-7.933	58.099	6.898	1.00	49.06
ATOM	202	N	GLN A	31	-8.972	58.807	5.025	1.00	45.74
ATOM	203	CA	GLN A	31	-7.820	58.573	4.164	1.00	42.76
ATOM	204	CB	GLN A	31	-8.188	58.781	2.701	1.00	40.15
ATOM	205	CG	GLN A	31	-9.129	57.723	2.175	1.00	43.01
ATOM	206	CD	GLN A	31	-9.468	57.922	0.715	1.00	48.15
ATOM	207	OE1	GLN A	31	-8.717	57.518	-0.166	1.00	52.25
ATOM	208	NE2	GLN A	31	-10.609	58.541	0.449	1.00	55.93
ATOM	209	C	GLN A	31	-6.675	59.494	4.568	1.00	41.22
ATOM	210	O	GLN A	31	-5.547	59.042	4.765	1.00	43.52
ATOM	211	N	ILE A	32	-6.977	60.778	4.732	1.00	37.48
ATOM	212	CA	ILE A	32	-5.972	61.746	5.138	1.00	31.13
ATOM	213	CB	ILE A	32	-6.581	63.140	5.280	1.00	26.04
ATOM	214	CG2	ILE A	32	-5.615	64.067	5.954	1.00	22.19
ATOM	215	CG1	ILE A	32	-6.987	63.663	3.904	1.00	25.80

ATOM	216	CD1	ILE	A	32	-7.608	65 039	3 924	1.00	27.42
ATOM	217	C	ILE	A	32	-5.343	61.308	6 458	1.00	34.56
ATOM	218	O	ILE	A	32	-4.123	61.345	6 606	1 00	38.92
ATOM	219	N	ASP	A	33	-6.169	60 833	7.387	1 00	36.94
ATOM	220	CA	ASP	A	33	-5.684	60 375	8.689	1.00	38.24
ATOM	221	CB	ASP	A	33	-6 850	59 928	9 588	1.00	44.05
ATOM	222	CG	ASP	A	33	-6 380	59 328	10.930	1.00	47.52
ATOM	223	OD1	ASP	A	33	-5 824	60.066	11 773	1.00	44.85
ATOM	224	OD2	ASP	A	33	-6 583	58 111	11.149	1.00	46.89
ATOM	225	C	ASP	A	33	-4 695	59.233	8.529	1.00	36.71
ATOM	226	O	ASP	A	33	-3.654	59.209	9 182	1.00	39.40
ATOM	227	N	ALA	A	34	-5.012	58.285	7 658	1.00	33.88
ATOM	228	CA	ALA	A	34	-4.129	57.148	7.445	1 00	34 39
ATOM	229	CB	ALA	A	34	-4.808	56 126	6 579	1 00	35 43
ATOM	230	C	ALA	A	34	-2 783	57.560	6 841	1 00	38 07
ATOM	231	O	ALA	A	34	-1.728	57.088	7 280	1.00	42 04
ATOM	232	N	ALA	A	35	-2.827	58.454	5.851	1.00	37.24
ATOM	233	CA	ALA	A	35	-1 596	58.933	5 197	1.00	34 56
ATOM	234	CB	ALA	A	35	-2 941	59.864	4.054	1.00	31.14
ATOM	235	C	ALA	A	35	-0 697	59 648	6 189	1.00	33.05
ATOM	236	O	ALA	A	35	0.485	59.347	6.295	1.00	36.62
ATOM	237	N	SER	A	36	-1.276	60.589	6.923	1.00	32.76
ATOM	238	CA	SER	A	36	-0 556	61 369	7.919	1 00	35 08
ATOM	239	CB	SER	A	36	-1 503	62.396	8 544	1 00	30 17
ATOM	240	OG	SER	A	36	-2 181	63.133	7 539	1 00	33 36
ATOM	241	C	SER	A	36	0.054	60.506	9.021	1.00	39.08
ATOM	242	O	SER	A	36	0 950	60 955	9 750	1.00	41.57
ATOM	243	N	ARG	A	37	-0 456	59.288	9 172	1.00	38 47
ATOM	244	CA	ARG	A	37	0 053	58 394	10.191	1.00	38 11
ATOM	245	CB	ARG	A	37	-1.095	57.702	10.908	1.00	40 18
ATOM	246	CG	ARG	A	37	-2.866	58.642	11.805	1 00	47 64
ATOM	247	CD	ARG	A	37	-3.157	58.021	12 262	1 00	55 80
ATOM	248	NE	ARG	A	37	-2.923	56.776	12.976	1 00	66 31
ATOM	249	CZ	ARG	A	37	-3 859	55.865	13.219	1.00	72.83
ATOM	250	NH1	ARG	A	37	-5.109	56.056	12.805	1.00	73.10
ATOM	251	NH2	ARG	A	37	-3 538	54.753	13.872	1.00	79.16
ATOM	252	C	ARG	A	37	1.035	57.393	9.627	1.00	38 74
ATOM	253	O	ARG	A	37	1.677	56.672	10 380	1.00	40.61
ATOM	254	N	ASP	A	38	1 151	57.349	8 305	1.00	40.43
ATOM	255	CA	ASP	A	38	2 086	56.440	7 658	1 00	41.47
ATOM	256	CB	ASP	A	38	1.435	55 783	6 437	1.00	49.45
ATOM	257	CG	ASP	A	38	2.199	54 556	5.951	1.00	58.59
ATOM	258	OD1	ASP	A	38	2.821	53 855	6.784	1.00	62.36
ATOM	259	OD2	ASP	A	38	2.162	54.281	4.732	1.00	62.50
ATOM	260	C	ASP	A	38	3.351	57.218	7 262	1.00	40.48
ATOM	261	O	ASP	A	38	4.213	57.461	8.105	1.00	36.69
ATOM	262	N	THR	A	39	3.449	57 618	5 991	1.00	41.01
ATOM	263	CA	THR	A	39	4.597	58.376	5 480	1.00	39.22
ATOM	264	CB	THR	A	39	4.675	58.298	3.948	1.00	39.18
ATOM	265	OG1	THR	A	39	3.363	58 473	3.393	1.00	44.29
ATOM	266	CG2	THR	A	39	5.221	56.968	3.519	1.00	43.28
ATOM	267	C	THR	A	39	4.497	59 847	5 850	1.00	37.79
ATOM	268	O	THR	A	39	5.505	60.538	5 973	1.00	41.79
ATOM	269	N	GLY	A	40	3.268	60.323	5 993	1.00	35.69
ATOM	270	CA	GLY	A	40	3.038	61.711	6 336	1.00	34.49
ATOM	271	C	GLY	A	40	2.842	62.524	5.078	1.00	32.99
ATOM	272	O	GLY	A	40	2.649	63.735	5.153	1.00	35.66
ATOM	273	N	PHE	A	41	2.867	61.842	3.932	1.00	32.44
ATOM	274	CA	PHE	A	41	2.713	62.465	2 617	1.00	30.35
ATOM	275	CB	PHE	A	41	3.986	62.260	1.780	1.00	23.42
ATOM	276	CG	PHE	A	41	5.094	63.225	2.094	1.00	19.36
ATOM	277	CD1	PHE	A	41	6.079	62.899	3 013	1.00	19.44
ATOM	278	CD2	PHE	A	41	5.161	64.455	1 454	1.00	20.61
ATOM	279	CE1	PHE	A	41	7.120	63.790	3 292	1.00	21.76
ATOM	280	CE2	PHE	A	41	6.192	65.350	1 723	1.00	19.48
ATOM	281	CZ	PHE	A	41	7.173	65.018	2 642	1.00	20.92
ATOM	282	C	PHE	A	41	1.558	61.855	1 840	1.00	30.54
ATOM	283	O	PHE	A	41	1.269	60.671	1 988	1.00	33.65
ATOM	284	N	PHE	A	42	0.900	62.662	1.016	1.00	29.43
ATOM	285	CA	PHE	A	42	-0.179	62.172	0.171	1.00	28.45
ATOM	286	CB	PHE	A	42	-1.473	61.872	0.953	1.00	28.60
ATOM	287	CG	PHE	A	42	-2.292	63.083	1.332	1.00	26.83
ATOM	288	CD1	PHE	A	42	-3.186	63.655	0.431	1.00	26.89

ATOM	289	CD2	PHE A	42	-2.218	63.612	2.613	1.00	28.60
ATOM	290	CE1	PHE A	42	-3.998	64.734	0.803	1.00	22.24
ATOM	291	CE2	PHE A	42	-3.030	64.692	2.993	1.00	28.04
ATOM	292	CZ	PHE A	42	-3.919	65.249	2.081	1.00	22.14
ATOM	293	C	PHE A	42	-0.416	63.122	-0.979	1.00	30.71
ATOM	294	O	PHE A	42	-0.046	64.297	-0.908	1.00	32.62
ATOM	295	N	TYR A	43	-0.911	62.580	-2.084	1.00	31.35
ATOM	296	CA	TYR A	43	-1.200	63.386	-3.257	1.00	27.25
ATOM	297	CB	TYR A	43	-0.851	62.641	-4.556	1.00	25.54
ATOM	298	CG	TYR A	43	0.573	62 844	-5.054	1.00	21.56
ATOM	299	CD1	TYR A	43	1.524	61 841	-4.942	1.00	19.07
ATOM	300	CE1	TYR A	43	2.835	62 034	-5.386	1.00	17.94
ATOM	301	CD2	TYR A	43	0.966	64 047	-5.628	1.00	23.58
ATOM	302	CE2	TYR A	43	2.272	64 246	-6 068	1.00	15.91
ATOM	303	CZ	TYR A	43	3.198	63 241	-5.946	1.00	16.09
ATOM	304	OH	TYR A	43	4.498	63 456	-6 375	1.00	15.37
ATOM	305	C	TYR A	43	-2.673	63.735	-3 249	1.00	29 51
ATOM	306	O	TYR A	43	-3.528	62.861	-3.163	1.00	26.39
ATOM	307	N	ALA A	44	-2.960	65 026	-3.252	1.00	32.50
ATOM	308	CA	ALA A	44	-4.327	65 497	-3.290	1.00	32.14
ATOM	309	CB	ALA A	44	-4.448	66 834	-2.586	1.00	32 97
ATOM	310	C	ALA A	44	-4.580	65 658	-4.769	1.00	32 97
ATOM	311	O	ALA A	44	-3.968	66 506	-5.414	1.00	33 03
ATOM	312	N	VAL A	45	-5.416	64.790	-5.317	1 00	33 76
ATOM	313	CA	VAL A	45	-5.741	64 824	-6.729	1 00	35 03
ATOM	314	CB	VAL A	45	-5.548	63 440	-7.353	1 00	36 59
ATOM	315	CG1	VAL A	45	-6.543	62 454	-6.770	1 00	40 19
ATOM	316	CG2	VAL A	45	-5.656	63 525	-8 861	1 00	47 08
ATOM	317	C	VAL A	45	-7.184	65 291	-6 866	1 00	36.63
ATOM	318	O	VAL A	45	-7.960	65 177	-5 917	1 00	42 25
ATOM	319	N	ASN A	46	-7.538	65 823	-8 034	1 00	36 71
ATOM	320	CA	ASN A	46	-8.883	66 349	-8 294	1 00	35.51
ATOM	321	CB	ASN A	46	-9.956	65.320	-7 942	1 00	42 00
ATOM	322	CG	ASN A	46	-10.436	64.547	-9.144	1.00	51.81
ATOM	323	OD1	ASN A	46	-11.513	64.813	-9 671	1.00	58.83
ATOM	324	ND2	ASN A	46	-9.641	63 582	-9.588	1 00	54 06
ATOM	325	C	ASN A	46	-9.121	67 618	-7 494	1 00	32 25
ATOM	326	O	ASN A	46	-10.206	67 848	-6 996	1.00	35.38
ATOM	327	N	HIS A	47	-8.093	68 452	-7 409	1 00	34 05
ATOM	328	CA	HIS A	47	-8.106	69 718	-6 659	1 00	34 39
ATOM	329	CB	HIS A	47	-6.674	70 088	-6 306	1 00	29 40
ATOM	330	CG	HIS A	47	-5.716	69 842	-7 425	1 00	26 18
ATOM	331	CD2	HIS A	47	-4.906	68 789	-7.686	1 00	27 13
ATOM	332	ND1	HIS A	47	-5.573	70 709	-8 486	1 00	29 56
ATOM	333	CE1	HIS A	47	-4.717	70 199	-9 355	1 00	29.92
ATOM	334	NE2	HIS A	47	-4.299	69 034	-8 894	1 00	29 91
ATOM	335	C	HIS A	47	-8.740	70.890	-7 397	1 00	35 30
ATOM	336	O	HIS A	47	-8.889	71 972	-6.825	1 00	36.82
ATOM	337	N	GLY A	48	-8.955	70.710	-8 700	1 00	36 56
ATOM	338	CA	GLY A	48	-9.578	71 732	-9.528	1 00	37 05
ATOM	339	C	GLY A	48	-8.759	72.959	-9 879	1 00	40 00
ATOM	340	O	GLY A	48	-9.321	74.004	-10.196	1 00	46.68
ATOM	341	N	ILE A	49	-7.440	72.819	-9 913	1 00	37.89
ATOM	342	CA	ILE A	49	-6.568	73 948	-10.220	1 00	36 05
ATOM	343	CB	ILE A	49	-5.546	74.191	-9 082	1 00	31 81
ATOM	344	CG2	ILE A	49	-4.522	75.255	-9 488	1 00	28 58
ATOM	345	CG1	ILE A	49	-6.287	74 596	-7 807	1 00	29 79
ATOM	346	CD1	ILE A	49	-5.425	74 629	-6 574	1 00	32.52
ATOM	347	C	ILE A	49	-5.815	73.686	-11.514	1 00	38 13
ATOM	348	O	ILE A	49	-5.297	72 581	-11 707	1 00	38 18
ATOM	349	N	ASN A	50	-5.749	74 701	-12 383	1 00	38 60
ATOM	350	CA	ASN A	50	-5.050	74 603	-13.663	1 00	38 30
ATOM	351	CB	ASN A	50	-5.453	75 726	-14.619	1 00	42 37
ATOM	352	CG	ASN A	50	-4.920	75.502	-16 033	1 00	46 03
ATOM	353	OD1	ASN A	50	-4.258	74 496	-16.314	1 00	46 67
ATOM	354	ND2	ASN A	50	-5.195	76 445	-16 922	1.00	49.68
ATOM	355	C	ASN A	50	-3.544	74.614	-13 439	1.00	38.19
ATOM	356	O	ASN A	50	-2.853	75 631	-13 581	1.00	36.43
ATOM	357	N	VAL A	51	-3.064	73.436	-13 086	1.00	39.42
ATOM	358	CA	VAL A	51	-1.676	73.165	-12.786	1.00	38.94
ATOM	359	CB	VAL A	51	-1.582	71.734	-12.182	1.00	36.89
ATOM	360	CG1	VAL A	51	-0.757	70.802	-13.040	1.00	39.25
ATOM	361	CG2	VAL A	51	-1.103	71.797	-10.756	1.00	37.13

ATOM	362	C	VAL	A	51	-0.804	73.346	-14.025	1.00	40.42
ATOM	363	O	VAL	A	51	0 370	73.688	-13.923	1.00	40.47
ATOM	364	N	GLN	A	52	-1 404	73 193	-15.198	1.00	43.48
ATOM	365	CA	GLN	A	52	-0.658	73 335	-16.439	1.00	46.46
ATOM	366	CB	GLN	A	52	-1.461	72 753	-17.607	1 00	54.80
ATOM	367	CG	GLN	A	52	-1.828	71 265	-17.427	1.00	64.12
ATOM	368	CD	GLN	A	52	-0.603	70 340	-17 338	1 00	70.98
ATOM	369	OE1	GLN	A	52	0.494	70.696	-17 774	1 00	73.27
ATOM	370	NE2	GLN	A	52	-0.799	69.140	-16.788	1 00	71.68
ATOM	371	C	GLN	A	52	-0.250	74.787	-16.694	1.00	42.90
ATOM	372	O	GLN	A	52	0.932	75.081	-16 876	1.00	42.08
ATOM	373	N	ARG	A	53	-1.212	75.704	-16 649	1.00	40.10
ATOM	374	CA	ARG	A	53	-0 902	77.119	-16.860	1.00	40.21
ATOM	375	CB	ARG	A	53	-2.161	77.981	-16.766	1 00	39.62
ATOM	376	CG	ARG	A	53	-1 896	79.468	-16 979	1 00	46.56
ATOM	377	CD	ARG	A	53	-3 084	80 302	-16.558	1 00	55.52
ATOM	378	NE	ARG	A	53	-3.456	80 002	-15.180	1.00	69.72
ATOM	379	CZ	ARG	A	53	-4.707	79.854	-14.750	1.00	75.43
ATOM	380	NH1	ARG	A	53	-5.728	79.988	-15.589	1.00	79.20
ATOM	381	NH2	ARG	A	53	-4.936	79.529	-13.485	1.00	80.30
ATOM	382	C	ARG	A	53	0.112	77 592	-15.828	1.00	40.89
ATOM	383	O	ARG	A	53	0.967	78.436	-16.103	1.00	42.68
ATOM	384	N	LEU	A	54	0 015	77.025	-14 617	1.00	40.83
ATOM	385	CA	LEU	A	54	0.906	77.354	-13.513	1 00	36.14
ATOM	386	CB	LEU	A	54	0.481	76 583	-12.263	1.00	36.52
ATOM	387	CG	LEU	A	54	1 431	76 620	-11.068	1 00	35.31
ATOM	388	CD1	LEU	A	54	1.581	78 057	-10.586	1 00	33.45
ATOM	389	CD2	LEU	A	54	0.904	75.710	-9.969	1 00	36.19
ATOM	390	C	LEU	A	54	2.380	77.073	-13.829	1 00	36.31
ATOM	391	O	LEU	A	54	3.231	77.935	-13.618	1.00	37.16
ATOM	392	N	SER	A	55	2 695	75 883	-14.335	1.00	34.98
ATOM	393	CA	SER	A	55	4.090	75.558	-14.645	1.00	36.10
ATOM	394	CB	SER	A	55	4 261	74 066	-14.929	1 00	32.09
ATOM	395	OG	SER	A	55	3.071	73 521	-15.455	1.00	41.05
ATOM	396	C	SER	A	55	4.618	76.377	-15.804	1.00	37.67
ATOM	397	O	SER	A	55	5.789	76 752	-15.825	1.00	41.07
ATOM	398	N	GLN	A	56	3 740	76 688	-16.744	1.00	37.35
ATOM	399	CA	GLN	A	56	4.105	77 460	-17.919	1 00	38.51
ATOM	400	CB	GLN	A	56	2.940	77 439	-18 902	1.00	46.09
ATOM	401	CG	GLN	A	56	3.138	78 188	-20.191	1.00	58.62
ATOM	402	CD	GLN	A	56	1 811	78.422	-20 902	1 00	71.60
ATOM	403	OE1	GLN	A	56	1 007	77.494	-21.071	1.00	75.28
ATOM	404	NE2	GLN	A	56	1 560	79 672	-21.296	1 00	74.89
ATOM	405	C	GLN	A	56	4 496	78.893	-17.560	1 00	36.41
ATOM	406	O	GLN	A	56	5.611	79 312	-17 848	1 00	35.97
ATOM	407	N	LYS	A	57	3 599	79.629	-16.905	1.00	35.19
ATOM	408	CA	LYS	A	57	3 869	81 015	-16.514	1 00	34.22
ATOM	409	CB	LYS	A	57	2 710	81.567	-15 693	1.00	35.10
ATOM	410	CG	LYS	A	57	1.443	81 768	-16.469	1.00	41.47
ATOM	411	CD	LYS	A	57	1 644	82.849	-17.492	1.00	49.86
ATOM	412	CE	LYS	A	57	0.507	82 868	-18 477	1.00	58.96
ATOM	413	NZ	LYS	A	57	0 740	83.914	-19.507	1 00	67.82
ATOM	414	C	LYS	A	57	5.147	81 106	-15.691	1.00	36.94
ATOM	415	O	LYS	A	57	5 963	82 014	-15.875	1 00	38.60
ATOM	416	N	THR	A	58	5 277	80 172	-14 753	1 00	37.65
ATOM	417	CA	THR	A	58	6.426	80.066	-13.865	1 00	35.48
ATOM	418	CB	THR	A	58	6 215	78 911	-12.846	1 00	36.09
ATOM	419	OG1	THR	A	58	5 257	79 317	-11.862	1 00	30.91
ATOM	420	CG2	THR	A	58	7 503	78 549	-12.142	1.00	43.44
ATOM	421	C	THR	A	58	7 696	79.833	-14.665	1 00	35.79
ATOM	422	O	THR	A	58	8 686	80.531	-14.463	1.00	37.07
ATOM	423	N	LYS	A	59	7 667	78 865	-15.577	1.00	38.20
ATOM	424	CA	LYS	A	59	8 832	78 573	-16.397	1.00	40.23
ATOM	425	CB	LYS	A	59	8.540	77.444	-17.391	1.00	46.70
ATOM	426	CG	LYS	A	59	9 744	77 071	-18.254	1.00	58.45
ATOM	427	CD	LYS	A	59	9 534	75 783	-19.053	1.00	69.21
ATOM	428	CE	LYS	A	59	10 831	75.350	-19.769	1.00	76.48
ATOM	429	NZ	LYS	A	59	10 728	74 041	-20.510	1.00	75.66
ATOM	430	C	LYS	A	59	9 199	79.846	-17.134	1.00	40.20
ATOM	431	O	LYS	A	59	10 364	80.239	-17.167	1.00	41.89
ATOM	432	N	GLU	A	60	8.186	80.531	-17.653	1.00	41.30
ATOM	433	CA	GLU	A	60	8.395	81.777	-18.379	1.00	42.90
ATOM	434	CB	GLU	A	60	7.059	82.362	-18.851	1.00	50.15

ATOM	435	CG	GLU A	60	6.405	81.626	-20.026	1.00	57.31
ATOM	436	CD	GLU A	60	5.215	82.383	-20.605	1.00	63.82
ATOM	437	OE1	GLU A	60	4.233	81.733	-21.027	1.00	68.21
ATOM	438	OE2	GLU A	60	5.259	83.633	-20.644	1.00	67.21
ATOM	439	C	GLU A	60	9.115	82 773	-17.484	1.00	39.96
ATOM	440	O	GLU A	60	10.147	83 324	-17.859	1.00	42.99
ATOM	441	N	PHE A	61	8.604	82 949	-16.274	1.00	35.82
ATOM	442	CA	PHE A	61	9.208	83.874	-15 325	1.00	34.12
ATOM	443	CB	PHE A	61	8.466	83.810	-13 978	1.00	30.54
ATOM	444	CG	PHE A	61	9.039	84.718	-12.918	1.00	25.45
ATOM	445	CD1	PHE A	61	8.905	86.093	-13.013	1.00	20.40
ATOM	446	CD2	PHE A	61	9.730	84.193	-11 835	1.00	23.25
ATOM	447	CE1	PHE A	61	9.449	86.928	-12.053	1.00	19 57
ATOM	448	CE2	PHE A	61	10.277	85.026	-10.875	1.00	22 69
ATOM	449	CZ	PHE A	61	10.133	86.399	-10.989	1.00	17 25
ATOM	450	C	PHE A	61	10 710	83.620	-15.115	1.00	32.38
ATOM	451	O	PHE A	61	11 536	84.499	-15.353	1.00	30.20
ATOM	452	N	HIS A	62	11.064	82.407	-14.714	1.00	34.34
ATOM	453	CA	HIS A	62	12 458	82.076	-14.436	1.00	37.14
ATOM	454	CB	HIS A	62	12 556	80.693	-13.779	1.00	32.21
ATOM	455	CG	HIS A	62	12.181	80.696	-12.331	1.00	31.98
ATOM	456	CD2	HIS A	62	11.234	80.007	-11.652	1.00	29.94
ATOM	457	ND1	HIS A	62	12.792	81.519	-11 410	1.00	28.87
ATOM	458	CE1	HIS A	62	12 234	81.344	-10 228	1.00	28.92
ATOM	459	NE2	HIS A	62	11 286	80.432	-10 347	1.00	29.72
ATOM	460	C	HIS A	62	13 437	82.193	-15 599	1 00	41.35
ATOM	461	O	HIS A	62	14 604	82.546	-15.405	1 00	40.97
ATOM	462	N	MET A	63	12 968	81.941	-16 809	1 00	43.02
ATOM	463	CA	MET A	63	13.867	82.018	-17.941	1 00	45.13
ATOM	464	CB	MET A	63	13 396	81.102	-19 070	1.00	51.35
ATOM	465	CG	MET A	63	13 180	79.653	-18 631	1.00	63.00
ATOM	466	SD	MET A	63	14 560	78.941	-17.665	1.00	73.59
ATOM	467	CE	MET A	63	15 229	77.786	-18 858	1.00	73.56
ATOM	468	C	MET A	63	14 052	83.438	-18 445	1.00	44.26
ATOM	469	O	MET A	63	15 126	83 781	-18 927	1.00	50 29
ATOM	470	N	SER A	64	13.041	84 283	-18 287	1.00	39.05
ATOM	471	CA	SER A	64	13.133	85.648	-18.782	1.00	36 67
ATOM	472	CB	SER A	64	11 798	86 062	-19 386	1.00	37 55
ATOM	473	OG	SER A	64	10 763	86 008	-18 428	1.00	43 44
ATOM	474	C	SER A	64	13 611	86 739	-17 837	1.00	39.95
ATOM	475	O	SER A	64	14.019	87 805	-18.296	1.00	45 98
ATOM	476	N	ILE A	65	13 486	86 531	-16 530	1.00	41.66
ATOM	477	CA	ILE A	65	13.914	87.547	-15 568	1.00	37.23
ATOM	478	CB	ILE A	65	13 477	87.209	-14 108	1.00	35.14
ATOM	479	CG2	ILE A	65	14 228	86 007	-13 559	1.00	26.54
ATOM	480	CG1	ILE A	65	13 725	88 412	-13 207	1 00	31.65
ATOM	481	CD1	ILE A	65	12 960	88.365	-11 914	1 00	37.39
ATOM	482	C	ILE A	65	15.420	87 732	-15 672	1.00	38.75
ATOM	483	O	ILE A	65	16.165	86.757	-15.710	1 00	43.09
ATOM	484	N	THR A	66	15.857	88.980	-15.785	1 00	38.80
ATOM	485	CA	THR A	66	17 278	89.281	-15 924	1.00	39.81
ATOM	486	CB	THR A	66	17.486	90 544	-16 776	1.00	40.56
ATOM	487	OG1	THR A	66	16 886	91 663	-16.113	1.00	47.40
ATOM	488	CG2	THR A	66	16 954	90 371	-18 139	1 00	41.17
ATOM	489	C	THR A	66	17 948	89.502	-14 580	1 00	39.84
ATOM	490	O	THR A	66	17 291	89 829	-13 597	1.00	46.85
ATOM	491	N	PRO A	67	19.279	89 365	-14 524	1.00	40.24
ATOM	492	CD	PRO A	67	20.152	88 850	-15 590	1.00	39.50
ATOM	493	CA	PRO A	67	20.037	89 557	-13 281	1 00	39.40
ATOM	494	CB	PRO A	67	21.482	89 273	-13 709	1 00	39.30
ATOM	495	CG	PRO A	67	21.459	89 446	-15.212	1 00	40.61
ATOM	496	C	PRO A	67	19 884	90 924	-12 604	1.00	39.27
ATOM	497	O	PRO A	67	19 934	91 012	-11 378	1.00	42.45
ATOM	498	N	GLU A	68	19 704	91 986	-13 387	1 00	37.98
ATOM	499	CA	GLU A	68	19 528	93 316	-12 811	1.00	36.08
ATOM	500	CB	GLU A	68	19.598	94 425	-13 865	1.00	44.41
ATOM	501	CG	GLU A	68	20 830	94.408	-14 745	1.00	56.01
ATOM	502	CD	GLU A	68	20 701	93.426	-15.897	1.00	62.86
ATOM	503	OE1	GLU A	68	19 776	93.599	-16.727	1.00	65.53
ATOM	504	OE2	GLU A	68	21.519	92 480	-15.972	1.00	66.08
ATOM	505	C	GLU A	68	18 166	93 349	-12.157	1.00	32.92
ATOM	506	O	GLU A	68	17 968	94 037	-11.158	1.00	37.34
ATOM	507	N	GLU A	69	17 217	92.633	-12.747	1.00	28.56

ATOM	508	CA	GLU A	69	15 877	92 560	-12 193	1 00	26.48
ATOM	509	CB	GLU A	69	14 927	92 889	-13 170	1.00	26.48
ATOM	510	CG	GLU A	69	14 696	92.647	-14 438	1.00	31.14
ATOM	511	CD	GLU A	69	13.480	92.145	-15 147	1.00	36 47
ATOM	512	OE1	GLU A	69	12.386	92.682	-14.875	1.00	41 34
ATOM	513	OE2	GLU A	69	13 612	91.195	-15 946	1.00	41 53
ATOM	514	C	GLU A	69	15 925	91.749	-10 900	1.00	26.61
ATOM	515	O	GLU A	69	15.268	92 086	-9 916	1.00	33.09
ATOM	516	N	LYS A	70	16.703	90 672	-10 902	1.00	23.31
ATOM	517	CA	LYS A	70	16 830	89.844	-9 719	1.00	18 07
ATOM	518	CB	LYS A	70	17.730	88 655	-10 000	1.00	16.10
ATOM	519	CG	LYS A	70	17.125	87.693	-10 978	1.00	16.50
ATOM	520	CD	LYS A	70	18.081	86.602	-11 323	1.00	19.40
ATOM	521	CE	LYS A	70	17.421	85 611	-12.243	1.00	23.23
ATOM	522	NZ	LYS A	70	18.372	84.538	-12.604	1.00	28.38
ATOM	523	C	LYS A	70	17.397	90 685	-8 596	1.00	22 66
ATOM	524	O	LYS A	70	16 836	90.725	-7 505	1.00	27.15
ATOM	525	N	TRP A	71	18.461	91 424	-8 891	1.00	21.96
ATOM	526	CA	TRP A	71	19.101	92.274	-7.897	1.00	22.52
ATOM	527	CB	TRP A	71	20.321	92.982	-8 494	1.00	29.42
ATOM	528	CG	TRP A	71	21.037	93.865	-7.506	1.00	20.03
ATOM	529	CD2	TRP A	71	21.800	93.441	-6.366	1.00	17.51
ATOM	530	CE2	TRP A	71	22.293	94.604	-5.736	1 00	15.91
ATOM	531	CE3	TRP A	71	22 103	92.194	-5.809	1 00	19.70
ATOM	532	CD1	TRP A	71	21 104	95.230	-7.524	1 00	18.18
ATOM	533	NE1	TRP A	71	21 859	95.680	-6.466	1.00	21.55
ATOM	534	CZ2	TRP A	71	23.089	94 559	-4.585	1.00	20.06
ATOM	535	CZ3	TRP A	71	22.897	92.147	-4.662	1 00	20.49
ATOM	536	CH2	TRP A	71	23.373	93.324	-4.061	1.00	20.53
ATOM	537	C	TRP A	71	18.123	93.299	-7 359	1.00	23.60
ATOM	538	O	TRP A	71	18.089	93 584	-6.155	1.00	24.12
ATOM	539	N	ASP A	72	17 327	93.860	-8.254	1.00	23.56
ATOM	540	CA	ASP A	72	16.358	94.859	7.860	1.00	27.03
ATOM	541	CB	ASP A	72	15 853	95.630	-9.083	1.00	34.54
ATOM	542	CG	ASP A	72	16 921	96.534	-9.692	1.00	40.55
ATOM	543	OD1	ASP A	72	18 116	96.375	-9.363	1.00	47.37
ATOM	544	OD2	ASP A	72	16.563	97.416	-10.502	1.00	50.79
ATOM	545	C	ASP A	72	15.208	94.309	-7.032	1.00	26.53
ATOM	546	O	ASP A	72	14.506	95 082	-6.384	1.00	33.99
ATOM	547	N	LEU A	73	15 055	92 989	-6.999	1.00	23.44
ATOM	548	CA	LEU A	73	13 998	92.353	-6 224	1.00	19 61
ATOM	549	CB	LEU A	73	13.219	91 372	-7 091	1.00	20 50
ATOM	550	CG	LEU A	73	12.333	91.920	-8 201	1.00	20 73
ATOM	551	CD1	LEU A	73	11.692	90.760	-8.945	1.00	10.89
ATOM	552	CD2	LEU A	73	11.280	92.830	-7.601	1.00	14.36
ATOM	553	C	LEU A	73	14 558	91.581	-5 049	1 00	19 51
ATOM	554	O	LEU A	73	13 811	91 098	-4.212	1 00	22.35
ATOM	555	N	ALA A	74	15 871	91 415	-5 019	1.00	20.26
ATOM	556	CA	ALA A	74	16 535	90.656	-3.965	1.00	18.26
ATOM	557	CB	ALA A	74	18.046	90.726	-4.146	1.00	17 07
ATOM	558	C	ALA A	74	16.163	91.106	-2.569	1.00	19.57
ATOM	559	O	ALA A	74	15 917	92.285	-2.344	1.00	17.06
ATOM	560	N	ILE A	75	16 115	90 157	-1 637	1.00	21.97
ATOM	561	CA	ILE A	75	15 811	90.457	-0.239	1.00	18 37
ATOM	562	CB	ILE A	75	15.337	89.202	0 514	1 00	15 88
ATOM	563	CG2	ILE A	75	14 056	88.700	-0.073	1 00	15 90
ATOM	564	CG1	ILE A	75	16 380	88.096	0 422	1.00	17.42
ATOM	565	CD1	ILE A	75	16 178	86.992	1 424	1 00	20 14
ATOM	566	C	ILE A	75	17 051	91.063	0.453	1 00	22 26
ATOM	567	O	ILE A	75	18.155	91.028	-0.093	1 00	24 15
ATOM	568	N	ARG A	76	16 866	91.598	1.656	1.00	23 62
ATOM	569	CA	ARG A	76	17 934	92.244	2.423	1 00	22 51
ATOM	570	CB	ARG A	76	17 382	92.683	3.776	1 00	25.41
ATOM	571	CG	ARG A	76	18 277	93.622	4.540	1.00	30.98
ATOM	572	CD	ARG A	76	17 650	93.958	5.878	1 00	39.61
ATOM	573	NE	ARG A	76	17 503	92.780	6.731	1 00	43.97
ATOM	574	CZ	ARG A	76	16.615	92.675	7.719	1 00	46.12
ATOM	575	NH1	ARG A	76	15 786	93.678	7.995	1 00	44.59
ATOM	576	NH2	ARG A	76	16.533	91.550	8.417	1.00	44.99
ATOM	577	C	ARG A	76	19.199	91.410	2.622	1.00	20.90
ATOM	578	O	ARG A	76	20.303	91.939	2.667	1.00	21.19
ATOM	579	N	ALA A	77	19.037	90.105	2.773	1.00	22.00
ATOM	580	CA	ALA A	77	20.175	89.219	2.962	1.00	20.40

ATOM	581	CB	ALA A	77	19.706	87.798	3.239	1.00	16.39
ATOM	582	C	ALA A	77	21.127	89.245	1.770	1.00	24.32
ATOM	583	O	ALA A	77	22.275	88.824	1.889	1.00	29.02
ATOM	584	N	TYR A	78	20.643	89.704	0.618	1.00	25.15
ATOM	585	CA	TYR A	78	21.471	89.795	-0.587	1.00	19.05
ATOM	586	CB	TYR A	78	20.810	89.103	-1.764	1.00	16.11
ATOM	587	CG	TYR A	78	20.748	87.628	-1.613	1.00	16.70
ATOM	588	CD1	TYR A	78	19.611	87.000	-1.114	1.00	15.71
ATOM	589	CE1	TYR A	78	19.542	85.626	-1.006	1.00	14.79
ATOM	590	CD2	TYR A	78	21.821	86.823	-1.987	1.00	17.98
ATOM	591	CE2	TYR A	78	21.762	85.458	-1.886	1.00	15.81
ATOM	592	CZ	TYR A	78	20.624	84.864	-1.394	1.00	19.26
ATOM	593	OH	TYR A	78	20.563	83.495	-1.336	1.00	27 92
ATOM	594	C	TYR A	78	21.735	91.233	-0.952	1.00	18 90
ATOM	595	O	TYR A	78	22.874	91.609	-1 178	1.00	24.83
ATOM	596	N	ASN A	79	20.672	92.025	-1 046	1.00	20 12
ATOM	597	CA	ASN A	79	20.778	93.442	-1 396	1.00	23 74
ATOM	598	CB	ASN A	79	19.767	93.794	-2.491	1.00	21 09
ATOM	599	CG	ASN A	79	19.985	95 173	-3.071	1.00	20 38
ATOM	600	OD1	ASN A	79	20.558	96 049	-2 437	1.00	24 59
ATOM	601	ND2	ASN A	79	19 511	95 378	-4 283	1.00	27.81
ATOM	602	C	ASN A	79	20 563	94 310	-0 161	1.00	26 18
ATOM	603	O	ASN A	79	19.442	94.645	0 206	1.00	28 37
ATOM	604	N	LYS A	80	21 668	94 695	0 452	1.00	28.39
ATOM	605	CA	LYS A	80	21 693	95 496	1 663	1.00	28 15
ATOM	606	CB	LYS A	80	23 145	95 869	1 926	1.00	30 31
ATOM	607	CG	LYS A	80	23 434	96.446	3 270	1.00	41 68
ATOM	608	CD	LYS A	80	24 934	96 530	3.472	1.00	49 85
ATOM	609	CE	LYS A	80	25.290	97 287	4 739	1.00	56 09
ATOM	610	NZ	LYS A	80	26.764	97 261	4 971	1.00	59 86
ATOM	611	C	LYS A	80	20 805	96.741	1 640	1.00	28.30
ATOM	612	O	LYS A	80	20.388	97.234	2 679	1.00	31 85
ATOM	613	N	GLU A	81	20.444	97.183	0.448	1 00	27.68
ATOM	614	CA	GLU A	81	19 631	98.377	0.245	1 00	27.82
ATOM	615	CB	GLU A	81	19 700	98 738	-1 245	1 00	26 85
ATOM	616	CG	GLU A	81	18 936	99 974	-1 667	1 00	25 54
ATOM	617	CD	GLU A	81	18.843	100 115	-3 173	1.00	27 23
ATOM	618	OE1	GLU A	81	18 424	101.187	-3 645	1.00	30 21
ATOM	619	OE2	GLU A	81	19 177	99 153	-3 892	1.00	35 72
ATOM	620	C	GLU A	81	18 163	98 261	0 685	1.00	28 54
ATOM	621	O	GLU A	81	17 592	99.190	1 260	1.00	32 85
ATOM	622	N	HIS A	82	17 544	97 125	0 406	1.00	28 51
ATOM	623	CA	HIS A	82	16 145	96.919	0 736	1.00	26 34
ATOM	624	CB	HIS A	82	15 547	95 839	-0.148	1.00	23.16
ATOM	625	CG	HIS A	82	15.992	95 898	-1 569	1.00	20 08
ATOM	626	CD2	HIS A	82	16 006	96 906	-2.467	1.00	14 88
ATOM	627	ND1	HIS A	82	16 428	94 781	-2.241	1.00	21.04
ATOM	628	CE1	HIS A	82	16.684	95 094	-3 493	1.00	20.58
ATOM	629	NE2	HIS A	82	16 433	96.382	-3 661	1.00	16 40
ATOM	630	C	HIS A	82	15 992	96 461	2.168	1.00	29.32
ATOM	631	O	HIS A	82	15 653	95.302	2.415	1.00	29.56
ATOM	632	N	GLN A	83	16 193	97.366	3 113	1.00	32 90
ATOM	633	CA	GLN A	83	16 084	97 006	4 517	1.00	36 06
ATOM	634	CB	GLN A	83	16 438	98.194	5 406	1.00	42 46
ATOM	635	CG	GLN A	83	17 942	98 406	5.566	1.00	54.39
ATOM	636	CD	GLN A	83	18 637	97.224	6.227	1.00	60 00
ATOM	637	OE1	GLN A	83	18 366	96.899	7.386	1.00	66.86
ATOM	638	NE2	GLN A	83	19 534	96 572	5.492	1.00	60 20
ATOM	639	C	GLN A	83	14 746	96 418	4 932	1.00	34 12
ATOM	640	O	GLN A	83	14 689	95 623	5.856	1.00	36 75
ATOM	641	N	ASP A	84	13 684	96 755	4.215	1.00	35.26
ATOM	642	CA	ASP A	84	12 353	96 260	4.546	1.00	35 02
ATOM	643	CB	ASP A	84	11 293	97.298	4.158	1.00	47 91
ATOM	644	CG	ASP A	84	11.437	98 611	4.925	1.00	61.72
ATOM	645	OD1	ASP A	84	11.115	99 673	4 344	1.00	68.07
ATOM	646	OD2	ASP A	84	11.863	98 587	6 104	1.00	69.22
ATOM	647	C	ASP A	84	11.987	94 912	3 931	1.00	30.42
ATOM	648	O	ASP A	84	10.890	94 402	4 158	1.00	31.96
ATOM	649	N	GLN A	85	12.881	94 331	3 146	1.00	23.30
ATOM	650	CA	GLN A	85	12.571	93 058	2 537	1.00	20.72
ATOM	651	CB	GLN A	85	12.946	93 059	1 068	1.00	20.88
ATOM	652	CG	GLN A	85	12.181	94.019	0.236	1.00	23.30
ATOM	653	CD	GLN A	85	12.434	93.811	-1.235	1.00	32.07

ATOM	654	OE1	GLN	A	85	12 670	94.762	-1.982	1.00	41.87
ATOM	655	NE2	GLN	A	85	12 378	92.565	-1.666	1.00	31.81
ATOM	656	C	GLN	A	85	13 286	91.930	3.242	1.00	22.01
ATOM	657	O	GLN	A	85	14 485	91.736	3 061	1.00	25 61
ATOM	658	N	VAL	A	86	12 551	91.171	4 038	1.00	21 04
ATOM	659	CA	VAL	A	86	13 151	90.063	4 758	1.00	20 72
ATOM	660	CB	VAL	A	86	12 835	90 127	6 271	1.00	23.91
ATOM	661	CG1	VAL	A	86	13 522	88.996	6 993	1.00	24 41
ATOM	662	CG2	VAL	A	86	13.272	91 445	6.856	1.00	24.17
ATOM	663	C	VAL	A	86	12.717	88 713	4 204	1.00	20.58
ATOM	664	O	VAL	A	86	13.554	87.851	3 990	1 00	29.31
ATOM	665	N	ARG	A	87	11.417	88 530	3 990	1 00	18 86
ATOM	666	CA	ARG	A	87	10 875	87 270	3 467	1.00	18.95
ATOM	667	CB	ARG	A	87	9.560	86.885	4 153	1 00	21 46
ATOM	668	CG	ARG	A	87	9.591	86 566	5.630	1 00	24.00
ATOM	669	CD	ARG	A	87	8.153	86 365	6.142	1 00	23.85
ATOM	670	NE	ARG	A	87	7.549	85.127	5.647	1 00	26.86
ATOM	671	CZ	ARG	A	87	6.252	84 833	5.742	1.00	24.59
ATOM	672	NH1	ARG	A	87	5.412	85 691	6.300	1.00	22.47
ATOM	673	NH2	ARG	A	87	5 803	83 654	5.333	1.00	22.94
ATOM	674	C	ARG	A	87	10.548	87 409	1 989	1.00	17 44
ATOM	675	O	ARG	A	87	10 947	86 591	1 181	1.00	20.34
ATOM	676	N	ALA	A	88	9.803	88 456	1.657	1.00	14.27
ATOM	677	CA	ALA	A	88	9 353	88 708	0 296	1 00	15.50
ATOM	678	CB	ALA	A	88	8 154	89.637	0 307	1.00	11.55
ATOM	679	C	ALA	A	88	10 413	89.247	-0 630	1 00	18.22
ATOM	680	O	ALA	A	88	11.122	90 190	-0 284	1 00	24.16
ATOM	681	N	GLY	A	89	10 461	88 688	-1 837	1 00	18.31
ATOM	682	CA	GLY	A	89	11 437	89.103	-2.825	1.00	18.37
ATOM	683	C	GLY	A	89	12.221	87.946	-3.422	1.00	21.93
ATOM	684	O	GLY	A	89	11 853	86.773	-3.262	1.00	23.18
ATOM	685	N	TYR	A	90	13 315	88.286	-4 103	1.00	21.46
ATOM	686	CA	TYR	A	90	14.178	87.314	-4 767	1.00	17.61
ATOM	687	CB	TYR	A	90	14 701	87 909	-6 098	1.00	14.11
ATOM	688	CG	TYR	A	90	14.847	86 895	-7 215	1 00	15.32
ATOM	689	CD1	TYR	A	90	13 827	86 705	-8.142	1.00	15.35
ATOM	690	CE1	TYR	A	90	13 900	85.686	-9.100	1.00	17.27
ATOM	691	CD2	TYR	A	90	15 963	86.050	-7.283	1.00	17.90
ATOM	692	CE2	TYR	A	90	16.047	85.031	-8 236	1.00	18.10
ATOM	693	CZ	TYR	A	90	15.010	84.855	-9.136	1.00	18.33
ATOM	694	OH	TYR	A	90	15.056	83 829	-10 056	1.00	29.46
ATOM	695	C	TYR	A	90	15 344	86 861	-3.881	1 00	18.14
ATOM	696	O	TYR	A	90	15.877	87 636	-3 089	1.00	19.67
ATOM	697	N	TYR	A	91	15.713	85.592	-4 013	1 00	20.08
ATOM	698	CA	TYR	A	91	16 819	84 976	-3 277	1 00	20.39
ATOM	699	CB	TYR	A	91	16 354	83.713	-2.542	1.00	20.44
ATOM	700	CG	TYR	A	91	15.353	83.965	-1.432	1.00	20.34
ATOM	701	CD1	TYR	A	91	14 116	84.566	-1.693	1 00	21.65
ATOM	702	CE1	TYR	A	91	13 211	84.819	-0 677	1.00	16.23
ATOM	703	CD2	TYR	A	91	15.651	83.622	-0 120	1.00	18.42
ATOM	704	CE2	TYR	A	91	14.753	83.867	0 898	1.00	20.40
ATOM	705	CZ	TYR	A	91	13.536	84.468	0.615	1.00	22.22
ATOM	706	OH	TYR	A	91	12.651	84.705	1 639	1.00	21.37
ATOM	707	C	TYR	A	91	17.819	84.603	-4.362	1.00	23.73
ATOM	708	O	TYR	A	91	17.583	83.687	-5 154	1.00	24.20
ATOM	709	N	LEU	A	92	18.894	85.374	-4.451	1.00	28.01
ATOM	710	CA	LEU	A	92	19.909	85.160	-5.476	1.00	24.96
ATOM	711	CB	LEU	A	92	20.857	86.362	-5.534	1.00	24.17
ATOM	712	CG	LEU	A	92	20.258	87.756	-5.635	1.00	19.59
ATOM	713	CD1	LEU	A	92	21.353	88.782	-5.696	1.00	23.44
ATOM	714	CD2	LEU	A	92	19.406	87.837	-6.850	1.00	22.64
ATOM	715	C	LEU	A	92	20.749	83.910	-5.283	1.00	25.80
ATOM	716	O	LEU	A	92	20.879	83.382	-4.174	1.00	25.07
ATOM	717	N	SER	A	93	21.310	83.440	-6.387	1.00	26.00
ATOM	718	CA	SER	A	93	22.210	82.307	-6.358	1.00	27.05
ATOM	719	CB	SER	A	93	22.218	81.584	-7.703	1.00	24.34
ATOM	720	OG	SER	A	93	22.434	82.479	-8.776	1.00	26.84
ATOM	721	C	SER	A	93	23.569	82.942	-6.087	1.00	27.46
ATOM	722	O	SER	A	93	23.776	84.125	-6.348	1.00	26.92
ATOM	723	N	ILE	A	94	24.487	82.178	-5.530	1.00	29.65
ATOM	724	CA	ILE	A	94	25.797	82.716	-5.234	1.00	31.96
ATOM	725	CB	ILE	A	94	26.106	82.624	-3.740	1.00	33.15
ATOM	726	CG2	ILE	A	94	27.467	83.228	-3.456	1.00	29.48

ATOM	727	CG1	ILE A	94	25.025	83.358	-2.946	1.00	33.35
ATOM	728	CD1	ILE A	94	25.091	83.120	-1.463	1.00	36.58
ATOM	729	C	ILE A	94	26.753	81.863	-6.027	1.00	34.38
ATOM	730	O	ILE A	94	26.946	80.691	-5.717	1.00	36.74
ATOM	731	N	PRO A	95	27 339	82.423	-7 080	1.00	38.50
ATOM	732	CD	PRO A	95	27 368	83.871	-7 350	1.00	40.61
ATOM	733	CA	PRO A	95	28 283	81.724	-7 947	1.00	40.90
ATOM	734	CB	PRO A	95	28 917	82.854	-8 745	1.00	45.71
ATOM	735	CG	PRO A	95	28 765	84.049	-7 829	1.00	45.59
ATOM	736	C	PRO A	95	29 309	80.929	-7 159	1 00	39.51
ATOM	737	O	PRO A	95	30 004	81.477	-6 310	1 00	42.47
ATOM	738	N	GLY A	96	29 327	79.625	-7 291	1 00	38.51
ATOM	739	CA	GLY A	96	30 259	78.752	-6 713	1 00	35.63
ATOM	740	C	GLY A	96	29 740	78.161	-5.424	1 00	37.97
ATOM	741	O	GLY A	96	30 126	77 062	-5 047	1 00	39.52
ATOM	742	N	LYS A	97	28 812	78 849	-4 777	1 00	35.33
ATOM	743	CA	LYS A	97	28 318	78 365	-3 504	1 00	34.40
ATOM	744	CB	LYS A	97	28 555	79 419	-2 435	1 00	42.78
ATOM	745	CG	LYS A	97	29 982	79.900	-2 352	1 00	54.46
ATOM	746	CD	LYS A	97	30 041	81.101	-1 428	1 00	65.72
ATOM	747	CE	LYS A	97	31 450	81 651	-1 284	1 00	73.04
ATOM	748	NZ	LYS A	97	31.498	82.894	-0 447	1 00	78.91
ATOM	749	C	LYS A	97	26 857	77 959	-3 450	1 00	32.83
ATOM	750	O	LYS A	97	26 501	77 068	-2 683	1 00	34.44
ATOM	751	N	LYS A	98	26 008	78 603	-4 243	1 00	26.60
ATOM	752	CA	LYS A	98	24 574	78 319	-4 215	1 00	22.39
ATOM	753	CB	LYS A	98	23 876	79 351	-3 319	1 00	23.74
ATOM	754	CG	LYS A	98	22.362	79 269	-3 276	1 00	22.19
ATOM	755	CD	LYS A	98	21 766	80.300	-2 335	1 00	22.81
ATOM	756	CE	LYS A	98	20 251	80 160	-2 241	1 00	22.30
ATOM	757	NZ	LYS A	98	19 547	80 977	-3 253	1 00	21.47
ATOM	758	C	LYS A	98	23 990	78.346	-5 614	1 00	21.39
ATOM	759	O	LYS A	98	24.076	79.355	-6 301	1.00	23.12
ATOM	760	N	ALA A	99	23 427	77 225	-6 044	1 00	21.69
ATOM	761	CA	ALA A	99	22 819	77 132	-7 369	1.00	23.49
ATOM	762	CB	ALA A	99	23 126	75 756	-7.983	1 00	21.77
ATOM	763	C	ALA A	99	21.301	77 449	-7.439	1 00	22.78
ATOM	764	O	ALA A	99	20 834	78 065	-8 399	1 00	25.07
ATOM	765	N	VAL A	100	20 547	77 040	-6 420	1 00	20.36
ATOM	766	CA	VAL A	100	19 106	77.274	-6 388	1 00	17.58
ATOM	767	CB	VAL A	100	18.462	76.528	-5.196	1 00	16.99
ATOM	768	CG1	VAL A	100	16 971	76.786	-5.130	1 00	14.01
ATOM	769	CG2	VAL A	100	18.722	75.044	-5.313	1 00	15.21
ATOM	770	C	VAL A	100	18.797	78.764	-6.277	1.00	20.86
ATOM	771	O	VAL A	100	19 574	79.506	-5.697	1 00	25.82
ATOM	772	N	GLU A	101	17 696	79.201	-6.885	1.00	20.04
ATOM	773	CA	GLU A	101	17 236	80.595	-6.829	1.00	17.64
ATOM	774	CB	GLU A	101	17 352	81.316	-8.185	1.00	22.33
ATOM	775	CG	GLU A	101	18 682	81.355	-8.862	1 00	27 61
ATOM	776	CD	GLU A	101	18.654	82.264	-10.048	1.00	28 27
ATOM	777	OE1	GLU A	101	19 711	82.803	-10.393	1.00	35 84
ATOM	778	OE2	GLU A	101	17 591	82.440	-10.656	1.00	33.44
ATOM	779	C	GLU A	101	15.734	80.502	-6.561	1 00	18.04
ATOM	780	O	GLU A	101	15.085	79.542	-6.977	1.00	20 27
ATOM	781	N	SER A	102	15.151	81.543	-5.989	1.00	15 18
ATOM	782	CA	SER A	102	13 727	81.512	-5.749	1.00	14 63
ATOM	783	CB	SER A	102	13 372	80.575	-4.599	1.00	16 17
ATOM	784	OG	SER A	102	14.095	80.881	-3.441	1.00	19 01
ATOM	785	C	SER A	102	13 172	82.883	-5.512	1.00	14.90
ATOM	786	O	SER A	102	13 919	83.805	-5.226	1.00	16.69
ATOM	787	N	PHE A	103	11 871	83.018	-5.753	1.00	16 08
ATOM	788	CA	PHE A	103	11 135	84.261	-5.579	1.00	14.05
ATOM	789	CB	PHE A	103	10 561	84.710	-6.928	1.00	11 82
ATOM	790	CG	PHE A	103	9 644	85.913	-6.849	1.00	14.83
ATOM	791	CD1	PHE A	103	10 149	87.189	-6.601	1.00	16.95
ATOM	792	CD2	PHE A	103	8.279	85.773	-7.081	1.00	11.21
ATOM	793	CE1	PHE A	103	9.295	88.309	-6.583	1.00	12.90
ATOM	794	CE2	PHE A	103	7.425	86.879	-7.065	1.00	10.94
ATOM	795	CZ	PHE A	103	7.936	88.146	-6.820	1.00	12.78
ATOM	796	C	PHE A	103	10.004	83.930	-4.607	1.00	14.85
ATOM	797	O	PHE A	103	9.249	82.981	-4.822	1.00	14.06
ATOM	798	N	CYS A	104	9.887	84.710	-3.543	1.00	14.45
ATOM	799	CA	CYS A	104	8.853	84.484	-2.548	1.00	14.61

ATOM	800	CB	CYS	A	104	9.509	84.235	-1.194	1.00	14 79
ATOM	801	SG	CYS	A	104	8.386	84 134	0 215	1.00	18 12
ATOM	802	C	CYS	A	104	7 896	85.662	-2 429	1.00	18.09
ATOM	803	O	CYS	A	104	8 322	86 821	-2 482	1.00	18 91
ATOM	804	N	TYR	A	105	6 600	85.367	-2.339	1 00	17 06
ATOM	805	CA	TYR	A	105	5.594	86 403	-2.161	1.00	13 87
ATOM	806	CB	TYR	A	105	4.941	86 845	-3.486	1.00	12.35
ATOM	807	CG	TYR	A	105	4 103	85 830	-4 234	1.00	14 43
ATOM	808	CD1	TYR	A	105	2.713	85.826	-4 110	1 00	9 55
ATOM	809	CE1	TYR	A	105	1 927	84.933	-4 832	1.00	7.61
ATOM	810	CD2	TYR	A	105	4.690	84 909	-5.112	1.00	11 05
ATOM	811	CE2	TYR	A	105	3.906	84.010	-5.846	1.00	13 52
ATOM	812	CZ	TYR	A	105	2.525	84 028	-5.699	1.00	15 44
ATOM	813	OH	TYR	A	105	1 733	83.129	-6 395	1 00	18 33
ATOM	814	C	TYR	A	105	4 576	85.967	-1.100	1 00	17.62
ATOM	815	O	TYR	A	105	4 412	84 773	-0 820	1 00	14.49
ATOM	816	N	LEU	A	106	3.991	86 954	-0 432	1 00	18 67
ATOM	817	CA	LEU	A	106	3.031	86 742	0.640	1.00	17.72
ATOM	818	CB	LEU	A	106	3.437	87.602	1.844	1.00	15 11
ATOM	819	CG	LEU	A	106	4 930	87 554	2.171	1.00	18.61
ATOM	820	CD1	LEU	A	106	5 237	88.376	3.384	1 00	18 40
ATOM	821	CD2	LEU	A	106	5.358	86.124	2.391	1 00	20.22
ATOM	822	C	LEU	A	106	1.594	87.078	0.237	1.00	19.75
ATOM	823	O	LEU	A	106	1.266	87.191	-0 947	1.00	19.55
ATOM	824	N	ASN	A	107	0 753	87.241	1.253	1 00	19 69
ATOM	825	CA	ASN	A	107	-0.659	87.563	1.122	1.00	16.25
ATOM	826	CB	ASN	A	107	-1.231	87.792	2 518	1 00	18 19
ATOM	827	CG	ASN	A	107	-2.738	87.979	2 530	1.00	24 35
ATOM	828	OD1	ASN	A	107	-3.332	88.525	1 591	1.00	22.21
ATOM	829	ND2	ASN	A	107	-3.362	87 551	3.518	1.00	16 86
ATOM	830	C	ASN	A	107	-0 817	88.812	0.279	1 00	15.33
ATOM	831	O	ASN	A	107	-0 332	89.888	0.634	1.00	16.38
ATOM	832	N	PRO	A	108	-1.497	88.686	-0 860	1.00	14 14
ATOM	833	CD	PRO	A	108	-1.973	87 430	-1 466	1.00	13.05
ATOM	834	CA	PRO	A	108	-1.712	89 818	-1.757	1.00	14.52
ATOM	835	CB	PRO	A	108	-2 552	89.206	-2.867	1 00	11 78
ATOM	836	CG	PRO	A	108	-2.018	87.779	-2.916	1.00	13.10
ATOM	837	C	PRO	A	108	-2 409	91.006	-1.113	1.00	15.10
ATOM	838	O	PRO	A	108	-2 295	92.126	-1.595	1.00	15 99
ATOM	839	N	ASN	A	109	-3.114	90.776	-0.014	1.00	16.27
ATOM	840	CA	ASN	A	109	-3 838	91.855	0.649	1.00	18.22
ATOM	841	CB	ASN	A	109	-5 005	91.304	1.461	1 00	17 89
ATOM	842	CG	ASN	A	109	-6.058	90.695	0.590	1 00	15 82
ATOM	843	OD1	ASN	A	109	-6 374	91.228	-0.475	1.00	18.28
ATOM	844	ND2	ASN	A	109	-6 578	89.549	1.001	1.00	14.24
ATOM	845	C	ASN	A	109	-2.990	92.759	1.511	1.00	19.06
ATOM	846	O	ASN	A	109	-3.467	93.786	1.978	1.00	22.19
ATOM	847	N	PHE	A	110	-1.762	92.349	1.791	1.00	17.26
ATOM	848	CA	PHE	A	110	-0.879	93.168	2.588	1.00	13.51
ATOM	849	CB	PHE	A	110	0.304	92.345	3.068	1.00	11.28
ATOM	850	CG	PHE	A	110	-0.054	91.343	4.110	1.00	14.89
ATOM	851	CD1	PHE	A	110	-1.296	91.384	4.727	1.00	14.80
ATOM	852	CD2	PHE	A	110	0.854	90.365	4.494	1.00	16.71
ATOM	853	CE1	PHE	A	110	-1.627	90.470	5.702	1.00	15.38
ATOM	854	CE2	PHE	A	110	0.532	89.440	5.474	1.00	14.69
ATOM	855	CZ	PHE	A	110	-0.710	89.495	6.082	1.00	18.74
ATOM	856	C	PHE	A	110	-0.404	94.363	1.787	1.00	16.88
ATOM	857	O	PHE	A	110	0.469	94.243	0.930	1.00	21.88
ATOM	858	N	THR	A	111	-1.032	95 509	2.004	1.00	18.68
ATOM	859	CA	THR	A	111	-0.625	96.718	1.304	1.00	16.37
ATOM	860	CB	THR	A	111	-1.764	97 305	0 482	1.00	15.54
ATOM	861	OG1	THR	A	111	-2.723	97 911	1.355	1.00	18.30
ATOM	862	CG2	THR	A	111	-2.423	96 221	-0 337	1.00	11.84
ATOM	863	C	THR	A	111	-0.219	97 692	2 389	1.00	18.43
ATOM	864	O	THR	A	111	-0.284	97 360	3 564	1.00	23.70
ATOM	865	N	PRO	A	112	0.229	98 895	2 023	1.00	21.65
ATOM	866	CD	PRO	A	112	0.707	99.351	0.703	1.00	15.84
ATOM	867	CA	PRO	A	112	0.626	99 845	3 069	1.00	23.93
ATOM	868	CB	PRO	A	112	1.273	100 969	2 272	1.00	21.58
ATOM	869	CG	PRO	A	112	1.847	100.236	1.079	1.00	19.10
ATOM	870	C	PRO	A	112	-0.507	100.371	3.954	1.00	28.77
ATOM	871	O	PRO	A	112	-0.245	100.991	4.981	1.00	34.33
ATOM	872	N	ASP	A	113	-1.756	100.137	3.557	1.00	30.89

ATOM	873	CA	ASP A	113	-2.908	100.608	4.325	1.00	29.23
ATOM	874	CB	ASP A	113	-4.095	100.876	3.403	1.00	33.62
ATOM	875	CG	ASP A	113	-3.740	101.759	2.229	1.00	39.32
ATOM	876	OD1	ASP A	113	-3.551	102.980	2.420	1.00	38.82
ATOM	877	OD2	ASP A	113	-3.659	101.220	1.107	1.00	41.64
ATOM	878	C	ASP A	113	-3.313	99.552	5.330	1.00	26.58
ATOM	879	O	ASP A	113	-4.020	99.831	6.288	1.00	30.47
ATOM	880	N	HIS A	114	-2.875	98.327	5.090	1.00	22.11
ATOM	881	CA	HIS A	114	-3.203	97.223	5.964	1.00	18.51
ATOM	882	CB	HIS A	114	-2.562	95.954	5.434	1.00	18.88
ATOM	883	CG	HIS A	114	-3.154	94.695	5.980	1.00	20.47
ATOM	884	CD2	HIS A	114	-3.955	93.771	5.401	1.00	20.61
ATOM	885	ND1	HIS A	114	-2.905	94.243	7.255	1.00	21.89
ATOM	886	CE1	HIS A	114	-3.527	93.092	7.440	1.00	20.69
ATOM	887	NE2	HIS A	114	-4.170	92.784	6.331	1.00	16.26
ATOM	888	C	HIS A	114	-2.682	97.529	7.347	1.00	20.91
ATOM	889	O	HIS A	114	-1.511	97.821	7.518	1.00	23.53
ATOM	890	N	PRO A	115	-3.535	97.414	8.365	1.00	23.07
ATOM	891	CD	PRO A	115	-4.933	96.973	8.311	1.00	24.88
ATOM	892	CA	PRO A	115	-3.148	97.688	9.745	1.00	24.93
ATOM	893	CB	PRO A	115	-4.411	97.334	10.525	1.00	27.48
ATOM	894	CG	PRO A	115	-5.094	96.342	9.652	1.00	24.00
ATOM	895	C	PRO A	115	-1.927	96.923	10.233	1.00	26.06
ATOM	896	O	PRO A	115	-1.127	97.456	10.991	1.00	32.32
ATOM	897	N	ARG A	116	-1.782	95.678	9.802	1.00	26.43
ATOM	898	CA	ARG A	116	-0.634	94.868	10.199	1.00	26.26
ATOM	899	CB	ARG A	116	-0.810	93.430	9.727	1.00	30.69
ATOM	900	CG	ARG A	116	-1.813	92.629	10.516	1.00	35.60
ATOM	901	CD	ARG A	116	-1.372	92.533	11.950	1.00	39.57
ATOM	902	NE	ARG A	116	-2.151	91.547	12.685	1.00	44.77
ATOM	903	CZ	ARG A	116	-2.021	91.314	13.988	1.00	47.07
ATOM	904	NH1	ARG A	116	-1.145	91.997	14.721	1.00	44.22
ATOM	905	NH2	ARG A	116	-2.758	90.379	14.556	1.00	46.39
ATOM	906	C	ARG A	116	0.681	95.416	9.653	1.00	27.56
ATOM	907	O	ARG A	116	1.727	95.273	10.276	1.00	28.41
ATOM	908	N	ILE A	117	0.624	96.021	8.473	1.00	28.17
ATOM	909	CA	ILE A	117	1.806	96.580	7.835	1.00	28.31
ATOM	910	CB	ILE A	117	1.584	96.734	6.307	1.00	24.00
ATOM	911	CG2	ILE A	117	2.790	97.357	5.644	1.00	23.25
ATOM	912	CG1	ILE A	117	1.315	95.372	5.668	1.00	20.98
ATOM	913	CD1	ILE A	117	2.506	94.482	5.596	1.00	16.97
ATOM	914	C	ILE A	117	2.140	97.930	8.490	1.00	34.06
ATOM	915	O	ILE A	117	3.308	98.237	8.742	1.00	40.01
ATOM	916	N	GLN A	118	1.111	98.716	8.797	1.00	34.32
ATOM	917	CA	GLN A	118	1.289	100.008	9.446	1.00	31.25
ATOM	918	CB	GLN A	118	-0.036	100.751	9.510	1.00	32.56
ATOM	919	CG	GLN A	118	-0.532	101.215	8.175	1.00	41.97
ATOM	920	CD	GLN A	118	-1.790	102.040	8.289	1.00	49.04
ATOM	921	OE1	GLN A	118	-2.349	102.203	9.374	1.00	54.55
ATOM	922	NE2	GLN A	118	-2.241	102.577	7.167	1.00	54.77
ATOM	923	C	GLN A	118	1.813	99.816	10.857	1.00	30.00
ATOM	924	O	GLN A	118	2.606	100.602	11.348	1.00	36.36
ATOM	925	N	ALA A	119	1.362	98.759	11.506	1.00	27.04
ATOM	926	CA	ALA A	119	1.801	98.470	12.851	1.00	23.94
ATOM	927	CB	ALA A	119	0.898	97.447	13.457	1.00	23.97
ATOM	928	C	ALA A	119	3.223	97.944	12.836	1.00	29.31
ATOM	929	O	ALA A	119	3.839	97.802	13.885	1.00	35.94
ATOM	930	N	LYS A	120	3.728	97.625	11.649	1.00	30.68
ATOM	931	CA	LYS A	120	5.068	97.075	11.497	1.00	31.26
ATOM	932	CB	LYS A	120	6.131	98.127	11.815	1.00	32.35
ATOM	933	CG	LYS A	120	6.210	99.208	10.756	1.00	41.07
ATOM	934	CD	LYS A	120	7.461	100.047	10.893	1.00	53.39
ATOM	935	CE	LYS A	120	7.720	100.864	9.621	1.00	60.71
ATOM	936	NZ	LYS A	120	9.046	101.563	9.644	1.00	65.99
ATOM	937	C	LYS A	120	5.271	95.796	12.321	1.00	30.22
ATOM	938	O	LYS A	120	6.266	95.633	13.014	1.00	34.12
ATOM	939	N	THR A	121	4.287	94.901	12.240	1.00	30.59
ATOM	940	CA	THR A	121	4.304	93.627	12.945	1.00	29.59
ATOM	941	CB	THR A	121	2.897	93.001	12.953	1.00	26.01
ATOM	942	OG1	THR A	121	1.948	93.993	13.347	1.00	29.93
ATOM	943	CG2	THR A	121	2.830	92.841	13.924	1.00	27.80
ATOM	944	C	THR A	21	5.238	92.685	12.203	1.00	31.22
ATOM	945	O	THR A	121	5.258	92.684	10.977	1.00	36.88

ATOM	946	N	PRO	A	122	6.016	91.867	12.918	1.00	31.48
ATOM	947	CD	PRO	A	122	6.173	91.788	14.375	1.00	30.51
ATOM	948	CA	PRO	A	122	6.936	90.939	12.260	1.00	29.39
ATOM	949	CB	PRO	A	122	7.519	90.162	13.428	1.00	28.00
ATOM	950	CG	PRO	A	122	7.524	91.147	14.508	1.00	28.89
ATOM	951	C	PRO	A	122	6.213	89.993	11.324	1.00	29.95
ATOM	952	O	PRO	A	122	5.017	89.759	11.499	1.00	33.22
ATOM	953	N	THR	A	123	6.957	89.422	10.373	1.00	30.79
ATOM	954	CA	THR	A	123	6.470	88.472	9.355	1.00	28.32
ATOM	955	CB	THR	A	123	5.859	87.189	9.961	1.00	30.03
ATOM	956	OG1	THR	A	123	4.648	87.498	10.661	1.00	35.13
ATOM	957	CG2	THR	A	123	6.835	86.507	10.897	1.00	31.48
ATOM	958	C	THR	A	123	5.505	89.028	8.309	1.00	27.79
ATOM	959	O	THR	A	123	5.164	88.310	7.377	1.00	29.06
ATOM	960	N	HIS	A	124	5.076	90.285	8.458	1.00	24.80
ATOM	961	CA	HIS	A	124	4.150	90.920	7.504	1.00	22.12
ATOM	962	CB	HIS	A	124	3.072	91.740	8.226	1.00	27.07
ATOM	963	CG	HIS	A	124	2.285	90.948	9.215	1.00	13.05
ATOM	964	CD2	HIS	A	124	1.035	90.435	9.145	1.00	18.78
ATOM	965	ND1	HIS	A	124	2.798	90.529	10.420	1.00	15.62
ATOM	966	CE1	HIS	A	124	1.907	89.785	11.044	1.00	17.88
ATOM	967	NE2	HIS	A	124	0.825	89.712	10.292	1.00	17.44
ATOM	968	C	HIS	A	124	4.941	91.837	6.592	1.00	21.71
ATOM	969	O	HIS	A	124	5.645	92.715	7.050	1.00	22.54
ATOM	970	N	GLU	A	125	4.819	91.632	5.295	1.00	21.78
ATOM	971	CA	GLU	A	125	5.538	92.456	4.339	1.00	20.92
ATOM	972	CB	GLU	A	125	6.787	91.730	3.852	1.00	23.07
ATOM	973	CG	GLU	A	125	8.023	91.998	4.651	1.00	24.04
ATOM	974	CD	GLU	A	125	9.169	91.132	4.222	1.00	24.79
ATOM	975	OE1	GLU	A	125	9.457	91.049	3.012	1.00	24.03
ATOM	976	OE2	GLU	A	125	9.793	90.539	5.107	1.00	31.23
ATOM	977	C	GLU	A	125	4.668	92.738	3.143	1.00	21.05
ATOM	978	O	GLU	A	125	3.660	92.080	2.930	1.00	24.62
ATOM	979	N	VAL	A	126	5.091	93.694	2.339	1.00	21.65
ATOM	980	CA	VAL	A	126	4.361	94.031	1.146	1.00	22.78
ATOM	981	CB	VAL	A	126	4.203	95.538	1.042	1.00	20.08
ATOM	982	CG1	VAL	A	126	3.508	95.900	-0.229	1.00	17.38
ATOM	983	CG2	VAL	A	126	3.405	96.028	2.228	1.00	20.49
ATOM	984	C	VAL	A	126	5.166	93.459	-0.019	1.00	25.89
ATOM	985	O	VAL	A	126	6.380	93.667	-0.099	1.00	30.48
ATOM	986	N	ASN	A	127	4.511	92.683	-0.880	1.00	21.77
ATOM	987	CA	ASN	A	127	5.174	92.053	-2.020	1.00	19.25
ATOM	988	CB	ASN	A	127	4.182	91.207	-2.830	1.00	18.25
ATOM	989	CG	ASN	A	127	3.724	89.985	-2.095	1.00	16.94
ATOM	990	OD1	ASN	A	127	4.459	89.445	-1.286	1.00	16.08
ATOM	991	ND2	ASN	A	127	2.512	89.528	-2.380	1.00	12.62
ATOM	992	C	ASN	A	127	5.857	93.007	-2.975	1.00	19.23
ATOM	993	O	ASN	A	127	5.436	94.150	-3.148	1.00	18.59
ATOM	994	N	VAL	A	128	6.948	92.525	-3.556	1.00	18.95
ATOM	995	CA	VAL	A	128	7.698	93.260	-4.561	1.00	23.17
ATOM	996	CB	VAL	A	128	9.228	93.403	-4.235	1.00	21.82
ATOM	997	CG1	VAL	A	128	9.427	94.284	-3.027	1.00	20.58
ATOM	998	CG2	VAL	A	128	9.880	92.055	-3.999	1.00	23.71
ATOM	999	C	VAL	A	128	7.494	92.408	-5.808	1.00	23.82
ATOM	1000	O	VAL	A	128	7.486	91.183	-5.730	1.00	23.35
ATOM	1001	N	TRP	A	129	7.312	93.050	-6.951	1.00	25.96
ATOM	1002	CA	TRP	A	129	7.066	92.319	-8.179	1.00	28.04
ATOM	1003	CB	TRP	A	129	5.604	92.476	-8.562	1.00	22.71
ATOM	1004	CG	TRP	A	129	4.646	91.925	-7.588	1.00	20.42
ATOM	1005	CD2	TRP	A	129	4.254	90.557	-7.467	1.00	17.81
ATOM	1006	CE2	TRP	A	129	3.222	90.505	-6.508	1.00	16.80
ATOM	1007	CE3	TRP	A	129	4.667	89.371	-8.084	1.00	17.14
ATOM	1008	CD1	TRP	A	129	3.873	92.629	-6.710	1.00	15.97
ATOM	1009	NE1	TRP	A	129	3.008	91.784	-6.063	1.00	17.97
ATOM	1010	CZ2	TRP	A	129	2.597	89.313	-6.155	1.00	19.47
ATOM	1011	CZ3	TRP	A	129	4.048	88.188	-7.734	1.00	16.93
ATOM	1012	CH2	TRP	A	129	3.024	88.167	-6.780	1.00	18.76
ATOM	1013	C	TRP	A	129	7.887	92.838	-9.336	1.00	30.23
ATOM	1014	O	TRP	A	129	8.323	93.985	-9.325	1.00	30.92
ATOM	1015	N	PRO	A	130	8.103	92.000	-10.361	1.00	32.08
ATOM	1016	CD	PRO	A	130	7.807	90.562	-10.498	1.00	31.53
ATOM	1017	CA	PRO	A	130	8.880	92.474	-11.503	1.00	33.41
ATOM	1018	CB	PRO	A	130	9.109	91.192	-12.308	1.00	31.40

ATOM	1019	CG	PRO A	130	7.926	90.364	-11 .986	1.00	28.64
ATOM	1020	C	PRO A	130	8.090	93.521	-12.298	1.00	35.25
ATOM	1021	O	PRO A	130	6.869	93.651	-12.146	1.00	36.95
ATOM	1022	N	ASP A	131	8.805	94.301	-13 100	1.00	38.98
ATOM	1023	CA	ASP A	131	8.185	95.329	-13.927	1.00	41.94
ATOM	1024	CB	ASP A	131	9.270	96.081	-14.699	1.00	49.89
ATOM	1025	CG	ASP A	131	8.713	97.168	-15 612	1.00	59.35
ATOM	1026	OD1	ASP A	131	7.519	97.540	-15.503	1.00	60.33
ATOM	1027	OD2	ASP A	131	9.499	97 667	-16 448	1.00	69.02
ATOM	1028	C	ASP A	131	7 160	94 732	-14.895	1.00	40 13
ATOM	1029	O	ASP A	131	7.444	93 761	-15 604	1 00	39 39
ATOM	1030	N	GLU A	132	5 983	95 343	-14 933	1.00	38.57
ATOM	1031	CA	GLU A	132	4.895	94 906	-15 796	1.00	41 66
ATOM	1032	CB	GLU A	132	3.675	95 805	-15 594	1 00	49.43
ATOM	1033	CG	GLU A	132	2 565	95 210	-14 742	1 00	63.43
ATOM	1034	CD	GLU A	132	1.767	94 123	-15 455	1.00	68.77
ATOM	1035	OE1	GLU A	132	1 390	93 130	-14 786	1.00	73.49
ATOM	1036	OE2	GLU A	132	1.502	94.268	-16.671	1.00	70.44
ATOM	1037	C	GLU A	132	5.249	94 919	-17.269	1 00	40.84
ATOM	1038	O	GLU A	132	4.925	93 984	-17 998	1.00	42.27
ATOM	1039	N	THR A	133	5 909	95.984	-17 709	1 00	40.91
ATOM	1040	CA	THR A	133	6 261	96.124	-19 114	1 00	42.12
ATOM	1041	CB	THR A	133	7 100	97.407	-19.373	1 00	43 93
ATOM	1042	OG1	THR A	133	8 431	97 217	-18 884	1 00	56 48
ATOM	1043	CG2	THR A	133	6 496	98 602	-18 650	1 00	42 47
ATOM	1044	C	THR A	133	7 045	94 908	-19.576	1 00	40.83
ATOM	1045	O	THR A	133	6.800	94.369	-20 650	1.00	45 82
ATOM	1046	N	LYS A	134	7 945	94 450	-18 717	1 00	40.62
ATOM	1047	CA	LYS A	134	8.799	93 312	-19 024	1.00	40 68
ATOM	1048	CB	LYS A	134	10 109	93 429	-18 233	1.00	44 31
ATOM	1049	CG	LYS A	134	10.852	94.742	-18.437	1.00	50 92
ATOM	1050	CD	LYS A	134	12.171	94.754	-17 681	1 00	56 36
ATOM	1051	CE	LYS A	134	12 883	96.096	-17 809	1.00	64 21
ATOM	1052	NZ	LYS A	134	14.159	96.104	-17 026	1 00	72.09
ATOM	1053	C	LYS A	134	8 176	91 950	-18.737	1.00	40.31
ATOM	1054	O	LYS A	134	8.563	90 955	-19 348	1 00	45 00
ATOM	1055	N	HIS A	135	7.278	91.875	-17.763	1.00	38 10
ATOM	1056	CA	HIS A	135	6 649	90.601	-17.425	1.00	34 82
ATOM	1057	CB	HIS A	135	7 200	90 072	-16.089	1 00	28 65
ATOM	1058	CG	HIS A	135	8 654	89.705	-16 124	1 00	21 40
ATOM	1059	CD2	HIS A	135	9 267	88 523	-16 373	1 00	22 41
ATOM	1060	ND1	HIS A	135	9 659	90 614	-15 880	1.00	21.96
ATOM	1061	CE1	HIS A	135	10.832	90 022	-15 978	1.00	21.23
ATOM	1062	NE2	HIS A	135	10.624	88 743	-16 276	1 00	26 04
ATOM	1063	C	HIS A	135	5 135	90 787	-17.335	1 00	37 00
ATOM	1064	O	HIS A	135	4.536	90 584	-16 271	1 00	36 99
ATOM	1065	N	PRO A	136	4.489	91 128	-18 465	1 00	38 00
ATOM	1066	CD	PRO A	136	5 065	91 093	-19 820	1 00	39 72
ATOM	1067	CA	PRO A	136	3.043	91.352	-18 545	1.00	35 57
ATOM	1068	CB	PRO A	136	2.801	91 478	-20.048	1.00	33.63
ATOM	1069	CG	PRO A	136	3.882	90 651	-20.639	1.00	35.65
ATOM	1070	C	PRO A	136	2.183	90 264	-17 935	1 00	33.54
ATOM	1071	O	PRO A	136	2 348	89 083	-18 231	1 00	35 53
ATOM	1072	N	GLY A	137	1 284	90.680	-17 053	1 00	33 66
ATOM	1073	CA	GLY A	137	0.379	89 753	-16 408	1 00	35 45
ATOM	1074	C	GLY A	137	0.946	88 810	-15 361	1 00	36 34
ATOM	1075	O	GLY A	137	0.212	87 982	-14.829	1.00	41.58
ATOM	1076	N	PHE A	138	2.224	88 926	-15.029	1 00	34 29
ATOM	1077	CA	PHE A	138	2.792	88.034	-14.022	1.00	32.30
ATOM	1078	CB	PHE A	138	4.315	88.175	-13 960	1 00	33.36
ATOM	1079	CG	PHE A	138	4.960	87 272	-12 959	1 00	29 73
ATOM	1080	CD1	PHE A	138	4.770	85 902	-13.026	1.00	31.50
ATOM	1081	CD2	PHE A	138	5.718	87 796	-11 924	1.00	30 02
ATOM	1082	CE1	PHE A	138	5.322	85.061	-12 070	1.00	32 69
ATOM	1083	CE2	PHE A	138	6.272	86.974	-10 965	1.00	30 29
ATOM	1084	CZ	PHE A	138	6.075	85.600	-11 035	1.00	33.63
ATOM	1085	C	PHE A	138	2.178	88.259	-12.639	1.00	31.05
ATOM	1086	O	PHE A	138	1.653	87.323	-12.029	1.00	29.39
ATOM	1087	N	GLN A	139	2.205	89.502	-12.169	1.00	26.99
ATOM	1088	CA	GLN A	139	1.662	89.815	-10.861	1.00	28.51
ATOM	1089	CB	GLN A	139	1.751	91.314	-10.581	1.00	23.97
ATOM	1090	CG	GLN A	139	1.090	91.725	-9.275	1.00	27.92
ATOM	1091	CD	GLN A	139	1.192	93.216	-8.982	1.00	32.88

ATOM	1092	OE1	GLN A	139	1 943	93.950	-9.632	1.00	32.97
ATOM	1093	NE2	GLN A	139	0 440	93.668	-7.987	1 00	31.33
ATOM	1094	C	GLN A	139	0 222	89 332	-10.734	1 00	33.84
ATOM	1095	O	GLN A	139	-0 126	88 663	-9.754	1.00	36 68
ATOM	1096	N	ASP A	140	-0 592	89.609	-11.752	1.00	37 09
ATOM	1097	CA	ASP A	140	-2 003	89.206	-11.747	1 00	35 96
ATOM	1098	CB	ASP A	140	-2 736	89.776	-12.972	1.00	40 62
ATOM	1099	CG	ASP A	140	-2 672	91.300	-13 044	1.00	49.63
ATOM	1100	OD1	ASP A	140	-3 391	91 955	-12 266	1.00	51.54
ATOM	1101	OD2	ASP A	140	-1.906	91.840	-13.875	1.00	56.38
ATOM	1102	C	ASP A	140	-2.140	87 684	-11 694	1.00	34.15
ATOM	1103	O	ASP A	140	-3.024	87.149	-11 023	1 00	35.48
ATOM	1104	N	PHE A	141	-1.258	86.981	-12 389	1 00	29.30
ATOM	1105	CA	PHE A	141	-1 305	85 530	-12 373	1.00	29 22
ATOM	1106	CB	PHE A	141	-0.296	84.942	-13 368	1 00	26.63
ATOM	1107	CG	PHE A	141	0 113	83.526	-13.051	1 00	32.93
ATOM	1108	CD1	PHE A	141	-0 721	82.456	-13 364	1 00	37 47
ATOM	1109	CD2	PHE A	141	1 312	83.263	-12.388	1 00	36 97
ATOM	1110	CE1	PHE A	141	-0 373	81.143	-13.016	1.00	37 55
ATOM	1111	CE2	PHE A	141	1.667	81.956	-12.035	1.00	37.91
ATOM	1112	CZ	PHE A	141	0.821	80.895	-12.349	1.00	36 70
ATOM	1113	C	PHE A	141	-0 971	85.033	-10 969	1.00	31.10
ATOM	1114	O	PHE A	141	-1.720	84.264	-10.369	1.00	34.39
ATOM	1115	N	ALA A	142	0 162	85 493	-10 454	1.00	27 56
ATOM	1116	CA	ALA A	142	0 657	85 091	-9 149	1.00	23.24
ATOM	1117	CB	ALA A	142	1 969	85 792	-8.880	1.00	26.02
ATOM	1118	C	ALA A	142	-0 317	85.313	-7.995	1 00	23 50
ATOM	1119	O	ALA A	142	-0.438	84.480	-7.094	1.00	23 30
ATOM	1120	N	GLU A	143	-1 013	86.437	-8 022	1 00	24.11
ATOM	1121	CA	GLU A	143	-1.969	86.750	-6.970	1.00	26.83
ATOM	1122	CB	GLU A	143	-2 403	88.211	-7.077	1.00	27.46
ATOM	1123	CG	GLU A	143	-1.262	89.196	-6.890	1.00	30.94
ATOM	1124	CD	GLU A	143	-1.733	90.618	-6.681	1.00	36.67
ATOM	1125	OE1	GLU A	143	-0.906	91.448	-6.250	1.00	40.24
ATOM	1126	OE2	GLU A	143	-2 921	90.916	-6 943	1.00	40.10
ATOM	1127	C	GLU A	143	-3.183	85.824	-7.018	1 00	29.25
ATOM	1128	O	GLU A	143	-3.640	85.318	-5.989	1.00	31 43
ATOM	1129	N	GLN A	144	-3.699	85.596	-8.219	1.00	30.46
ATOM	1130	CA	GLN A	144	-4.843	84.725	-8 392	1 00	28.86
ATOM	1131	CB	GLN A	144	-5.275	84.696	-9 858	1.00	38.80
ATOM	1132	CG	GLN A	144	-6.529	83.852	-10 139	1.00	58.07
ATOM	1133	CD	GLN A	144	-7.754	84.269	-9.309	1.00	67.99
ATOM	1134	OE1	GLN A	144	-8.542	83.420	-8.876	1.00	72.49
ATOM	1135	NE2	GLN A	144	-7.922	85.573	-9.099	1.00	74.56
ATOM	1136	C	GLN A	144	-4 449	83.339	-7 938	1.00	25.81
ATOM	1137	O	GLN A	144	-5 201	82.669	-7.239	1 00	30.61
ATOM	1138	N	TYR A	145	-3.259	82.905	-8.335	1 00	26.62
ATOM	1139	CA	TYR A	145	-2.788	81.590	-7.944	1.00	22.39
ATOM	1140	CB	TYR A	145	-1.393	81.286	-8.505	1.00	21.02
ATOM	1141	CG	TYR A	145	-0 895	79.930	-8 047	1.00	23.34
ATOM	1142	CD1	TYR A	145	-1 603	78.770	-8.356	1.00	21.49
ATOM	1143	CE1	TYR A	145	-1.224	77.533	-7.846	1.00	19.67
ATOM	1144	CD2	TYR A	145	0 221	79.814	-7 219	1.00	23.57
ATOM	1145	CE2	TYR A	145	0 607	78.579	-6 705	1.00	20.74
ATOM	1146	CZ	TYR A	145	-0.122	77.449	-7.024	1.00	20.82
ATOM	1147	OH	TYR A	145	0 250	76.231	-6 518	1.00	24.24
ATOM	1148	C	TYR A	145	-2.791	81.487	-6 422	1.00	22.08
ATOM	1149	O	TYR A	145	-3.231	80.482	-5.875	1.00	24.79
ATOM	1150	N	TYR A	146	-2 360	82.546	-5.740	1.00	20.10
ATOM	1151	CA	TYR A	146	-2 329	82 552	-4.283	1.00	16.74
ATOM	1152	CB	TYR A	146	-1.933	83 931	-3.773	1.00	15.16
ATOM	1153	CG	TYR A	146	-1 652	83 991	-2.289	1.00	19 44
ATOM	1154	CD1	TYR A	146	-0 345	84 050	-1.807	1.00	19 08
ATOM	1155	CE1	TYR A	146	-0.088	84 132	-0.458	1.00	17 67
ATOM	1156	CD2	TYR A	146	-2 691	84 023	-1.364	1.00	18 53
ATOM	1157	CE2	TYR A	146	-2 438	84 103	-0.002	1.00	17 70
ATOM	1158	CZ	TYR A	146	-1 137	84 161	0.437	1.00	19.52
ATOM	1159	OH	TYR A	146	-0 875	84 226	1.774	1.00	25 01
ATOM	1160	C	TYR A	146	-3.704	82 193	-3.770	1.00	17.31
ATOM	1161	O	TYR A	146	-3.859	81 274	-2.967	1.00	21.09
ATOM	1162	N	TRP A	147	-4.713	82.882	-4.284	1.00	17.15
ATOM	1163	CA	TRP A	147	-6.087	82.620	-3.881	1.00	17.97
ATOM	1164	CB	TRP A	147	-6.988	83.752	-4.363	1.00	14.43

ATOM	1165	CG	TRP	A	147	-6.580	85.045	-3.742	1.00	16.44
ATOM	1166	CD2	TRP	A	147	-6.371	85.292	-2.353	1.00	15.61
ATOM	1167	CE2	TRP	A	147	-5.855	86.588	-2.222	1.00	13.55
ATOM	1168	CE3	TRP	A	147	-6.556	84.520	-1.195	1.00	13.91
ATOM	1169	CD1	TRP	A	147	-6.209	86.192	-4.389	1.00	17.35
ATOM	1170	NE1	TRP	A	147	-5.760	87.222	-3.482	1.00	16.82
ATOM	1171	CZ2	TRP	A	147	-5.526	87.238	-0.999	1.00	15.71
ATOM	1172	CZ3	TRP	A	147	-6.225	85.066	0.023	1.00	13.54
ATOM	1173	CH2	TRP	A	147	-5.714	86.365	0.114	1.00	14.81
ATOM	1174	C	TRP	A	147	-6.589	81 238	-4.308	1.00	19.27
ATOM	1175	O	TRP	A	147	-7.401	80 620	-3.611	1.00	19.35
ATOM	1176	N	ASP	A	148	-6.059	80 731	-5.416	1.00	18.47
ATOM	1177	CA	ASP	A	148	-6.416	79 405	-5.904	1.00	19.12
ATOM	1178	CB	ASP	A	148	-5.801	79 141	-7 275	1.00	24 71
ATOM	1179	CG	ASP	A	148	-6.709	79 536	-8 404	1.00	26 35
ATOM	1180	OD1	ASP	A	148	-7.852	79.946	-8 136	1.00	32 40
ATOM	1181	OD2	ASP	A	148	-6.284	79 423	-9 569	1.00	32.06
ATOM	1182	C	ASP	A	148	-5.973	78.328	-4 927	1 00	18 33
ATOM	1183	O	ASP	A	148	-6.797	77.536	-4 486	1.00	23 56
ATOM	1184	N	VAL	A	149	-4.679	78 276	-4 603	1 00	18 47
ATOM	1185	CA	VAL	A	149	-4.193	77.281	-3.647	1.00	15 91
ATOM	1186	CB	VAL	A	149	-2.678	77 225	-3.513	1.00	14.54
ATOM	1187	CG1	VAL	A	149	-2.136	76 214	-4 447	1 00	17 43
ATOM	1188	CG2	VAL	A	149	-2.056	78 590	-3 729	1 00	16 13
ATOM	1189	C	VAL	A	149	-4 757	77 549	-2.271	1 00	18 11
ATOM	1190	O	VAL	A	149	-4 897	76.633	-1.467	1 00	21 98
ATOM	1191	N	PHE	A	150	-5 032	78 814	-1.979	1.00	20.18
ATOM	1192	CA	PHE	A	150	-5 629	79 173	-0.703	1 00	21.84
ATOM	1193	CB	PHE	A	150	-5.931	80 666	-0.669	1.00	29 11
ATOM	1194	CG	PHE	A	150	-6 442	81 152	0.651	1.00	22 85
ATOM	1195	CD1	PHE	A	150	-5 572	81 689	1.586	1 00	22 65
ATOM	1196	CD2	PHE	A	150	-7 794	81 091	0.955	1 00	26.06
ATOM	1197	CE1	PHE	A	150	-6 045	82 158	2.800	1 00	26.82
ATOM	1198	CE2	PHE	A	150	-8.274	81 561	2.171	1 00	22.46
ATOM	1199	CZ	PHE	A	150	-7 400	82 093	3.091	1 00	25.45
ATOM	1200	C	PHE	A	150	-6 933	78 382	-0.581	1 00	24.16
ATOM	1201	O	PHE	A	150	-7 214	77.769	0.453	1.00	28.22
ATOM	1202	N	GLY	A	151	-7.715	78.379	-1.656	1 00	22.56
ATOM	1203	CA	GLY	A	151	-8 970	77 659	-1.656	1 00	20.54
ATOM	1204	C	GLY	A	151	-8.761	76.182	-1.417	1.00	21.70
ATOM	1205	O	GLY	A	151	-9.504	75 565	-0.654	1 00	25.57
ATOM	1206	N	LEU	A	152	-7.745	75 610	-2.049	1.00	18 26
ATOM	1207	CA	LEU	A	152	-7.460	74.193	-1.876	1.00	29 08
ATOM	1208	CB	LEU	A	152	-6.304	73.770	-2.782	1.00	29.81
ATOM	1209	CG	LEU	A	152	-5.838	72.318	-2.680	1.00	19.38
ATOM	1210	CD1	LEU	A	152	-6.969	71.381	-3.103	1.00	26.96
ATOM	1211	CD2	LEU	A	152	-4.615	72.127	-3.538	1.00	11.13
ATOM	1212	C	LEU	A	152	-7.093	73.916	-0.425	1.00	24.24
ATOM	1213	O	LEU	A	152	-7.667	73.032	0.219	1.00	26.47
ATOM	1214	N	SER	A	153	-6.141	74.682	0.095	1.00	24.56
ATOM	1215	CA	SER	A	153	-5.687	74.517	1.468	1.00	22.73
ATOM	1216	CB	SER	A	153	-4.591	75.528	1.770	1.00	21.22
ATOM	1217	OG	SER	A	153	-3.572	75.448	0.787	1.00	21.77
ATOM	1218	C	SER	A	153	-6.842	74.665	2.444	1.00	22.43
ATOM	1219	O	SER	A	153	-7.041	73.823	3.316	1.00	24.75
ATOM	1220	N	SER	A	154	-7.642	75.698	2.245	1.00	22.50
ATOM	1221	CA	SER	A	154	-8.792	75.950	3.088	1.00	25.72
ATOM	1222	CB	SER	A	154	-9.588	77.108	2.497	1.00	25.08
ATOM	1223	OG	SER	A	154	-10.672	77.472	3.328	1.00	38.08
ATOM	1224	C	SER	A	154	-9.662	74.688	3.218	1.00	29.51
ATOM	1225	O	SER	A	154	-10.140	74.356	4.310	1.00	33.28
ATOM	1226	N	ALA	A	155	-9.786	73.941	2.121	1.00	31.53
ATOM	1227	CA	ALA	A	155	-10.582	72.713	2.099	1.00	29.45
ATOM	1228	CB	ALA	A	155	-11.038	72.396	0.696	1.00	30.93
ATOM	1229	C	ALA	A	155	-9.846	71 523	2.683	1.00	28.62
ATOM	1230	O	ALA	A	155	-10.473	70 657	3.281	1.00	32.89
ATOM	1231	N	LEU	A	156	-8.530	71 455	2.485	1.00	28.48
ATOM	1232	CA	LEU	A	156	-7.739	70 355	3.032	1.00	23.61
ATOM	1233	CB	LEU	A	156	-6.323	70 368	2 476	1.00	23.88
ATOM	1234	CG	LEU	A	156	-6.043	69 867	1.061	1.00	20.69
ATOM	1235	CD1	LEU	A	156	-4.587	70 132	0.729	1.00	20.27
ATOM	1236	CD2	LEU	A	156	-6.325	68 394	0.958	1.00	20.84
ATOM	1237	C	LEU	A	156	-7.688	70.488	4.547	1.00	25.37

ATOM	1238	O	LEU A	156	-7.558	69 490	5.262	1 00	26.18
ATOM	1239	N	LEU A	157	-7.773	71 726	5.036	1 00	25.81
ATOM	1240	CA	LEU A	157	-7.770	71 981	6 474	1 00	25.36
ATOM	1241	CB	LEU A	157	-7 557	73.466	6 775	1 00	19.73
ATOM	1242	CG	LEU A	157	-6.135	74 027	6 673	1.00	16.53
ATOM	1243	CD1	LEU A	157	-6 111	75 418	7 270	1 00	17.68
ATOM	1244	CD2	LEU A	157	-5 165	73 150	7 431	1 00	15.33
ATOM	1245	C	LEU A	157	-9 076	71.470	7 107	1 00	29.31
ATOM	1246	O	LEU A	157	-9 111	71 079	8 279	1 00	32.51
ATOM	1247	N	LYS A	158	-10 161	71.500	6 341	1 00	33.23
ATOM	1248	CA	LYS A	158	-11 442	70 982	6 814	1.00	31.84
ATOM	1249	CB	LYS A	158	-12 553	71 355	5.837	1 00	33.31
ATOM	1250	CG	LYS A	158	-12.780	72.845	5.745	1.00	34.09
ATOM	1251	CD	LYS A	158	-13 850	73 167	4.738	1 00	41.31
ATOM	1252	CE	LYS A	158	-14.186	74 649	4.754	1 00	47.04
ATOM	1253	NZ	LYS A	158	-15 362	74.923	3.886	1 00	56.43
ATOM	1254	C	LYS A	158	-11 289	69.460	6.905	1.00	30.71
ATOM	1255	O	LYS A	158	-11 770	68.836	7 848	1.00	34.49
ATOM	1256	N	GLY A	159	-10.570	68 884	5.942	1.00	30.71
ATOM	1257	CA	GLY A	159	-10.313	67.453	5.930	1 00	28.93
ATOM	1258	C	GLY A	159	-9.447	67 040	7.111	1 00	30.81
ATOM	1259	O	GLY A	159	-9 690	66 003	7.732	1 00	34.67
ATOM	1260	N	TYR A	160	-8 440	67 851	7.431	1 00	28.73
ATOM	1261	CA	TYR A	160	-7 556	67.575	8 556	1 00	29.15
ATOM	1262	CB	TYR A	160	-6.378	68.554	8.556	1 00	29.86
ATOM	1263	CG	TYR A	160	-5.181	68.055	7 780	1 00	28.35
ATOM	1264	CD1	TYR A	160	-4 828	68.607	6.543	1.00	26.01
ATOM	1265	CE1	TYR A	160	-3 727	68 124	5.830	1 00	25.65
ATOM	1266	CD2	TYR A	160	-4.412	67 017	8.279	1.00	26.25
ATOM	1267	CE2	TYR A	160	-3.321	66 530	7.584	1.00	26.20
ATOM	1268	CZ	TYR A	160	-2.977	67.076	6 365	1.00	28.06
ATOM	1269	OH	TYR A	160	-1.884	66.546	5.711	1.00	25.91
ATOM	1270	C	TYR A	160	-8 313	67 646	9 884	1 00	32.18
ATOM	1271	O	TYR A	160	-8 034	66 884	10.812	1.00	33.45
ATOM	1272	N	ALA A	161	-9.262	68 571	9.976	1 00	33.22
ATOM	1273	CA	ALA A	161	-10.074	68.734	11 180	1 00	30.35
ATOM	1274	CB	ALA A	161	-10.995	69 919	11 021	1 00	30.11
ATOM	1275	C	ALA A	161	-10 890	67 470	11.433	1.00	31.40
ATOM	1276	O	ALA A	161	-10 863	66.911	12.525	1.00	32.99
ATOM	1277	N	LEU A	162	-11 593	67 012	10.405	1.00	30.20
ATOM	1278	CA	LEU A	162	-12.405	65.813	10 501	1 00	31.99
ATOM	1279	CB	LEU A	162	-13.156	65.587	9 186	1 00	32.01
ATOM	1280	CG	LEU A	162	-14.116	66.719	8 801	1 00	33.82
ATOM	1281	CD1	LEU A	162	-14.867	66.349	7.545	1.00	34.17
ATOM	1282	CD2	LEU A	162	-15.096	66 997	9.933	1 00	34.51
ATOM	1283	C	LEU A	162	-11.580	64.580	10.877	1 00	32.42
ATOM	1284	O	LEU A	162	-12.002	63 767	11 .696	1 00	35.19
ATOM	1285	N	ALA A	163	-10.396	64 453	10.291	1.00	34.99
ATOM	1286	CA	ALA A	163	-9.504	63.325	10 573	1 00	32.51
ATOM	1287	CB	ALA A	163	-8.289	63.395	9 670	1.00	28.78
ATOM	1288	C	ALA A	163	-9.061	63 273	12.038	1.00	30.64
ATOM	1289	O	ALA A	163	-8.745	62.217	12 571	1 00	30.60
ATOM	1290	N	LEU A	164	-8.995	64.428	12.674	1 00	29.60
ATOM	1291	CA	LEU A	164	-8.578	64.478	14 054	1 00	30.80
ATOM	1292	CB	LEU A	164	-7.639	65.666	14 274	1 00	30.81
ATOM	1293	CG	LEU A	164	-6.284	65.550	13.570	1.00	29.00
ATOM	1294	CD1	LEU A	164	-5.583	66.875	13 576	1.00	30.09
ATOM	1295	CD2	LEU A	164	-5.434	64.509	14.245	1.00	28.45
ATOM	1296	C	LEU A	164	-9.778	64.529	14.993	1.00	34.67
ATOM	1297	O	LEU A	164	-9.633	64.811	16.179	1.00	37.15
ATOM	1298	N	GLY A	165	-10.964	64.258	14 455	1.00	35.40
ATOM	1299	CA	GLY A	165	-12.172	64.258	15.265	1.00	34.11
ATOM	1300	C	GLY A	165	-12.637	65.606	15.781	1.00	35.01
ATOM	1301	O	GLY A	165	-13.465	65.680	16.694	1.00	38.99
ATOM	1302	N	LYS A	166	-12.111	66.678	15.208	1.00	34.42
ATOM	1303	CA	LYS A	166	-12.490	68.021	15.619	1.00	34.45
ATOM	1304	CB	LYS A	166	-11.267	68.924	15.571	1.00	31.93
ATOM	1305	CG	LYS A	166	-10.232	68.560	16.594	1.00	32.57
ATOM	1306	CD	LYS A	166	-10.711	68.973	17.956	1.00	34.75
ATOM	1307	CE	LYS A	166	-9.756	68.522	19.022	1.00	38.74
ATOM	1308	NZ	LYS A	166	-10.078	69.161	20.313	1.00	40.84
ATOM	1309	C	LYS A	166	-13.557	68.535	14.666	1.00	37.47
ATOM	1310	O	LYS A	166	-13.825	67.901	13.642	1.00	41.52

ATOM	1311	N	GLU A	167	-14.189	69.660	14.994	1.00	38.98
ATOM	1312	CA	GLU A	167	-15.202	70.205	14.094	1.00	41.09
ATOM	1313	CB	GLU A	167	-15.947	71.398	14.713	1.00	45.19
ATOM	1314	CG	GLU A	167	-15.110	72.638	15.025	1.00	55.15
ATOM	1315	CD	GLU A	167	-14.565	72.661	16.448	1.00	61.94
ATOM	1316	OE1	GLU A	167	-14.118	73.742	16.887	1.00	62.92
ATOM	1317	OE2	GLU A	167	-14.584	71.611	17.131	1.00	64.60
ATOM	1318	C	GLU A	167	-14.525	70.605	12.780	1.00	41.39
ATOM	1319	O	GLU A	167	-13.339	70.935	12.761	1.00	41.98
ATOM	1320	N	GLU A	168	-15.285	70.581	11.692	1.00	39.45
ATOM	1321	CA	GLU A	168	-14.779	70.918	10.365	1.00	38.77
ATOM	1322	CB	GLU A	168	-15.943	70.959	9.387	1.00	40.01
ATOM	1323	CG	GLU A	168	-15.535	70.844	7.951	1.00	42.60
ATOM	1324	CD	GLU A	168	-16.721	70.635	7 056	1.00	45 09
ATOM	1325	OE1	GLU A	168	-17.408	71.626	6 740	1.00	51.44
ATOM	1326	OE2	GLU A	168	-16.979	69.477	6 677	1.00	50.69
ATOM	1327	C	GLU A	168	-13.965	72.212	10 255	1.00	37.65
ATOM	1328	O	GLU A	168	-12.966	72.270	9.533	1.00	37.39
ATOM	**1329**	**N**	**ASN A**	**169**	**-14.389**	**73.247**	**10.965**	**1.00**	**34.88**
ATOM	1330	CA	ASN A	169	-13.696	74.527	10 925	1.00	31.36
ATOM	1331	CB	ASN A	169	-14.710	75.654	10 976	1.00	38.29
ATOM	1332	CG	ASN A	169	-15.529	75.726	9 732	1.00	46.39
ATOM	1333	OD1	ASN A	169	-14.993	75.919	8 646	1.00	52.41
ATOM	1334	ND2	ASN A	169	-16.833	75.544	9 865	1.00	52.70
ATOM	1335	C	ASN A	169	-12.677	74.717	12.029	1.00	29.02
ATOM	1336	O	ASN A	169	-12.264	75.839	12.318	1.00	25.13
ATOM	1337	N	PHE A	170	-12.236	73.618	12.617	1.00	29.52
ATOM	1338	CA	PHE A	170	-11.276	73.687	13 702	1.00	30 89
ATOM	1339	CB	PHE A	170	-10.938	72.275	14 191	1.00	34.08
ATOM	1340	CG	PHE A	170	-10.030	72.248	15 377	1.00	38.01
ATOM	1341	CD1	PHE A	170	-10.418	72.827	16 575	1.00	41.53
ATOM	1342	CD2	PHE A	170	-8.778	71.658	15 293	1.00	39.11
ATOM	1343	CE1	PHE A	170	-9.571	72.824	17.675	1.00	40 36
ATOM	1344	CE2	PHE A	170	-7.925	71.649	16.385	1.00	41 21
ATOM	1345	CZ	PHE A	170	-8.326	72.235	17 580	1.00	42.47
ATOM	1346	C	PHE A	170	-10.012	74.464	13.305	1.00	32.24
ATOM	1347	O	PHE A	170	-9.496	75.255	14.102	1.00	32 82
ATOM	1348	N	PHE A	171	-9.537	74.269	12 072	1.00	30 18
ATOM	1349	CA	PHE A	171	-8.338	74.959	11.595	1.00	25.80
ATOM	1350	CB	PHE A	171	-7.436	74 018	10 780	1 00	21.23
ATOM	1351	CG	PHE A	171	-6.801	72 922	11.584	1 00	17 74
ATOM	1352	CD1	PHE A	171	-6.984	71 592	11.232	1 00	19 14
ATOM	1353	CD2	PHE A	171	-6.028	73 212	12 699	1 00	20 58
ATOM	1354	CE1	PHE A	171	-6 409	70 559	11.986	1 00	19 44
ATOM	1355	CE2	PHE A	171	-5 449	72 188	13.457	1 00	19.74
ATOM	1356	CZ	PHE A	171	-5 644	70 861	13 095	1 00	18 77
ATOM	1357	C	PHE A	171	-8 720	76.142	10.722	1.00	27 98
ATOM	1358	O	PHE A	171	-8 301	77 282	10 968	1.00	26 96
ATOM	1359	N	ALA A	172	-9 573	75 874	9 737	1 00	27 10
ATOM	1360	Q	ALA A	172	-10.009	76.880	8 770	1.00	23.60
ATOM	1361	CB	ALA A	172	-10 996	76 276	7.798	1.00	20.83
ATOM	1362	C	ALA A	172	-10.542	78 191	9 310	1 00	25.20
ATOM	1363	O	ALA A	172	-10.477	79 204	8 623	1 00	27.68
ATOM	1364	N	ARG A	173	-11 044	78 195	10 540	1.00	27.56
ATOM	1365	CA	MG A	173	-11 573	79 429	11.098	1 00	28 04
ATOM	1366	CB	ARG A	173	-12 374	79.170	12.377	1.00	29 47
ATOM	1367	CG	ARG A	173	-11 559	79 001	13.633	1 00	35 23
ATOM	1368	CD	MG A	173	-12 452	78 858	14 868	1 00	40 18
ATOM	1369	NE	MG A	173	-12 898	77.482	15.106	1.00	44 83
ATOM	1370	CZ	ARG A	173	-14 162	77.074	15 017	1.00	48 14
ATOM	1371	NH1	MG A	173	-15.122	77.934	14 695	1.00	48 64
ATOM	1372	NH2	MG A	173	-14 468	75.800	15 240	1.00	44 20
ATOM	1373	C	MG A	173	-10 433	80.401	11.355	1.00	30 23
ATOM	1374	O	ARG A	173	-10.657	81.591	11 584	1.00	32 24
ATOM	1375	N	HIS A	174	-9 206	79.889	11 314	1.00	28 30
ATOM	1376	CA	HIS A	174	-8 023	80.713	11 537	1.00	28 03
ATOM	1377	CB	HIS A	174	-7.051	79.999	12 473	1.00	25 87
ATOM	1378	CG	HIS A	174	-7 622	79.688	13 816	1.00	26 33
ATOM	1379	CD2	HIS A	174	-8 121	78.536	14.326	1.00	28 81
ATOM	1380	ND1	HIS A	174	-7.705	80.623	14 826	1.00	27 96
ATOM	1381	CE1	HIS A	174	-8.228	80.059	15 900	1.00	28 08
ATOM	1382	NE2	HIS A	174	-8.488	78.793	15 624	1.00	27 09
ATOM	1383	C	HIS A	174	-7.305	81.064	10 235	1.00	27 63

ATOM	1384	O	HIS A	174	-6.371	81 865	10 240	1.00	31.26
ATOM	1385	N	PHE A	175	-7.734	80 442	9 138	1.00	26.90
ATOM	1386	CA	PHE A	175	-7.165	80.631	7.801	1.00	22.15
ATOM	1387	CB	PHE A	175	-7 222	79 289	7 074	1.00	21.26
ATOM	1388	CG	PHE A	175	-6 293	79 176	5.911	1.00	23.40
ATOM	1389	CD1	PHE A	175	-6 652	78.420	4.803	1.00	20.93
ATOM	1390	CD2	PHE A	175	-5 046	79 781	5 931	1.00	19.53
ATOM	1391	CE1	PHE A	175	-5 789	78 266	3 741	1.00	19.79
ATOM	1392	CE2	PHE A	175	-4 170	79.630	4 866	1.00	19 63
ATOM	1393	CZ	PHE A	175	-4 545	78 870	3 770	1.00	19 09
ATOM	1394	C	PHE A	175	-8.030	81.655	7 071	1.00	23.58
ATOM	1395	O	P8E A	175	-9 032	81.299	6 443	1.00	25 37
ATOM	1396	N	LYS A	176	-7 636	82.923	7.136	1.00	22.96
ATOM	1397	CA	LYS A	176	-8 412	84.004	6 529	1.00	26.79
ATOM	1398	CB	LYS A	176	-8.991	84 922	7.619	1.00	32.23
ATOM	1399	CG	LYS A	176	-9 711	84 185	8.752	1.00	37 22
ATOM	1400	CD	LYS A	176	-10.312	85.139	9.782	1.00	45.14
ATOM	1401	CE	LYS A	176	-9 271	86.065	10 408	1.00	51 76
ATOM	1402	NZ	LYS A	176	-8 282	85.352	11.277	1.00	54 44
ATOM	1403	C	LYS A	176	-7.624	84.842	5.529	1.00	26.95
ATOM	1404	O	LYS A	176	-6.447	85.150	5.736	1.00	29 87
ATOM	1405	N	PRO A	177	-8 308	85 327	4.485	1 00	24.40
ATOM	1406	CD	PRO A	177	-9.714	85.067	4 146	1.00	20.13
ATOM	1407	CA	PRO A	177	-7.685	86 133	3 445	1 00	19.31
ATOM	1408	CB	PRO A	177	-8 838	86.376	2.481	1 00	16.22
ATOM	1409	CG	PRO A	177	-9 687	85.187	2.664	1 00	13.22
ATOM	1410	C	PRO A	177	-7.084	87.434	3.903	1.00	21.14
ATOM	1411	O	PRO A	177	-6.096	87 883	3 349	1.00	25.46
ATOM	1412	N	ASP A	178	-7.660	88 049	4.917	1.00	26.69
ATOM	1413	CA	ASP A	178	-7.145	89.341	5 355	1.00	30.90
ATOM	1414	CB	ASP A	178	-8 220	90.162	6.073	1.00	40.73
ATOM	1415	CG	ASP A	178	-8 927	89.377	7.153	1.00	58.65
ATOM	1416	OD1	ASP A	178	-9.660	88.411	6.813	1.00	67.55
ATOM	1417	OD2	ASP A	178	-8.754	89 731	8.344	1.00	69.29
ATOM	1418	C	ASP A	178	-5.891	89 303	6.183	1.00	25.93
ATOM	1419	O	ASP A	178	-5 154	90.282	6.225	1.00	27.92
ATOM	1420	N	ASP A	179	-5.620	88.180	6.828	1.00	20.77
ATOM	1421	CA	ASP A	179	-4.432	88.129	7 645	1.00	20.37
ATOM	1422	CB	ASP A	179	-4 790	88.332	9.120	1.00	24.28
ATOM	1423	CG	ASP A	179	-5 553	87.157	9 717	1.00	28.49
ATOM	1424	OD1	ASP A	179	-5.957	86.249	8.967	1.00	32.76
ATOM	1425	OD2	ASP A	179	-5.750	87.134	10 953	1.00	34.31
ATOM	1426	C	ASP A	179	-3 550	86.912	7 499	1.00	20.24
ATOM	1427	O	ASP A	179	-2 568	86.807	8 224	1.00	22.73
ATOM	1428	N	THR A	180	-3 870	85.996	6.587	1.00	18.73
ATOM	1429	CA	THR A	180	-3 035	84.809	6 453	1.00	19.30
ATOM	1430	CB	THR A	180	-3.533	83.818	5 372	1.00	20.49
ATOM	1431	OG1	THR A	180	-2.592	82.741	5 254	1.00	20.62
ATOM	1432	CG2	THR A	180	-3.657	84.488	4.024	1.00	18.20
ATOM	1433	C	THR A	180	-1.577	85.144	6.173	1.00	22.74
ATOM	1434	O	THR A	180	-1.269	86.060	5.407	1.00	23.45
ATOM	1435	N	LEU A	181	-0.689	84.402	6.826	1.00	22.30
ATOM	1436	CA	LEU A	181	0.752	84.558	6.661	1 00	19 63
ATOM	1437	CB	LEU A	181	1.450	84.460	8.023	1 00	11.22
ATOM	1438	CG	LEU A	181	1.280	85.655	8.947	1 00	8 88
ATOM	1439	CD1	LEU A	181	1.760	85.318	10.332	1 00	7 59
ATOM	1440	CD2	LEU A	181	2.041	86.823	8.395	1 00	9 34
ATOM	1441	C	LEU A	181	1.315	83.488	5.702	1.00	19.45
ATOM	1442	O	LEU A	181	2.524	83.287	5.629	1 00	22.17
ATOM	1443	N	ALA A	182	0.441	82.775	5.003	1 00	15.84
ATOM	1444	CA	ALA A	182	0.886	81.749	4.072	1 00	13.71
ATOM	1445	CB	ALA A	182	-0.306	81.111	3.410	1 00	15.01
ATOM	1446	C	ALA A	182	1.797	82.379	3.017	1.00	16.85
ATOM	1447	O	ALA A	182	1.690	83.571	2.723	1.00	15.28
ATOM	1448	N	SER A	183	2.679	81.583	2.429	1.00	15.86
ATOM	1449	CA	SER A	183	3.584	82.108	1.416	1.00	14.12
ATOM	1450	CB	SER A	183	4.947	82.430	2.039	1.00	12.59
ATOM	1451	OG	SER A	183	5.585	81 250	2.497	1.00	13.59
ATOM	1452	C	SER A	183	3.759	81 130	0.257	1.00	13.98
ATOM	1453	O	SER A	183	3.602	79.923	0.422	1.00	17.17
ATOM	1454	N	VAL A	184	4.008	81.674	-0.931	1.00	15.35
ATOM	1455	CA	VAL A	184	4.241	80.885	-2.133	1.00	13.86
ATOM	1456	CB	VAL A	184	3.366	81.361	-3.335	1.00	13.35

ATOM	1457	CG1	VAL A	184	3.625	80.500	-4.554	1.00	11.12
ATOM	1458	CG2	VAL A	184	1.907	81.283	-2.994	1.00	14.34
ATOM	1459	C	VAL A	184	5.698	81.161	-2.479	1.00	13.94
ATOM	1460	O	VAL A	184	6.123	82.314	-1.459	1.00	15.07
ATOM	1461	N	VAL A	185	6.469	80.107	-2.722	1.00	16.12
ATOM	1462	CA	VAL A	185	7.871	80.237	-3 095	1.00	18 01
ATOM	1463	CB	VAL A	185	8 818	79.516	-2 096	1.00	19 45
ATOM	1464	CG1	VAL A	185	10 262	79.683	-1 528	1.00	14 07
ATOM	1465	CG2	VAL A	185	8 629	80.054	-0 708	1.00	17 49
ATOM	1466	C	VAL A	185	8 039	79.551	-4 438	1.00	18 98
ATOM	1467	O	VAL A	185	7 660	78.391	-4 585	1.00	20 19
ATOM	1468	N	LEU A	186	8 541	80.282	-5 428	1.00	22 23
ATOM	1469	CA	LEU A	186	8 782	79.717	-6 760	1.00	22 67
ATOM	1470	CB	LEU A	186	8 468	80.748	-7 861	1.00	17 46
ATOM	1471	CG	LEU A	186	7 117	81.480	-7 844	1.00	17 76
ATOM	1472	CD1	LEU A	186	6 993	82.315	-9 092	1.00	19.25
ATOM	1473	CD2	LEU A	186	5 970	80.514	-7 761	1.00	12.57
ATOM	1474	C	LEU A	186	10.261	79.325	-6.800	1.00	21.43
ATOM	1475	O	LEU A	186	11 124	80 169	-7 058	1 00	21.60
ATOM	1476	N	ILE A	187	10 555	78 065	-6 500	1 00	18 26
ATOM	1477	CA	ILE A	187	11 929	77 586	-6 477	1 00	18 51
ATOM	1478	CB	ILE A	187	12 068	76 373	-5 547	1 00	17 33
ATOM	1479	CG2	ILE A	187	13 524	75 915	-5 484	1 00	17 55
ATOM	1480	CG1	ILE A	187	11 560	76 727	-4 152	1 00	14 78
ATOM	1481	CD1	ILE A	187	11 608	75 582	-3 201	1 00	12 56
ATOM	1482	C	ILE A	187	12.421	77.183	-7 858	1.00	24 55
ATOM	1483	O	ILE A	187	11.688	76.567	-8 632	1.00	28.10
ATOM	1484	N	ARG A	188	13.671	77 509	-8 158	1.00	27.00
ATOM	1485	CA	ARG A	188	14.258	77 160	-9 447	1.00	27.28
ATOM	1486	CB	ARG A	188	14 659	78 405	-10 241	1 00	25.39
ATOM	1487	CG	ARG A	188	15 481	78 037	-11 466	1.00	26.11
ATOM	1488	CD	ARG A	188	16.122	79.207	-12 169	1.00	26 92
ATOM	1489	NE	ARG A	188	16.656	78 756	-13 448	1 00	33 43
ATOM	1490	CZ	ARG A	188	17.555	79 406	-14.176	1 00	37 61
ATOM	1491	NH1	M G A	188	18.054	80 567	-13.779	1 00	40 25
ATOM	1492	NH2	ARG A	188	17 945	78.890	-15.327	1 00	45 39
ATOM	1493	C	ARG A	188	15.494	76 291	-9.302	1.00	27.56
ATOM	1494	O	ARG A	188	16 462	76.678	-8.644	1 00	26.16
ATOM	1495	N	TYR A	189	15.463	75 120	-9 921	1 00	28 98
ATOM	1496	Q	TYR A	189	16 605	74 221	-9 902	1 00	30 25
ATOM	1497	CB	TYR A	189	16 166	72 799	-9 600	1 00	28.57
ATOM	1498	CG	TYR A	189	15.715	72 610	-8 179	1 00	27.58
ATOM	1499	CD1	TYR A	189	14.363	72 586	-7 862	1 00	30 42
ATOM	1500	CE1	TYR A	189	13 933	72 371	-6 555	1 00	32 46
ATOM	1501	CD2	TYR A	189	16.639	72 419	-7 154	1 00	25 30
ATOM	1502	CE2	TYR A	189	16 224	72.206	-5.846	1 00	27 43
ATOM	1503	CZ	TYR A	189	14 866	72 182	-5.553	1.00	21 28
ATOM	1504	OH	TYR A	189	14.434	71 980	-4.262	1.00	37 45
ATOM	1505	C	TYR A	189	17.225	74 335	-11 293	1 00	30.75
ATOM	1506	O	TYR A	189	16.643	73 905	-12.278	1 00	31.49
ATOM	1507	N	PRO A	190	18.396	74.974	-11.388	1 00	29.84
ATOM	1508	CD	PRO A	190	19.157	75.502	-10.238	1.00	29.04
ATOM	1509	CA	PRO A	190	19.131	75.192	-12.631	1.00	29 41
ATOM	1510	CB	PRO A	190	20.122	76.271	-12 222	1 00	30.04
ATOM	1511	CG	PRO A	190	20.508	75.816	-10 845	1 00	27.63
ATOM	1512	C	PRO A	190	19.899	74.005	-13.163	1.00	29.09
ATOM	1513	O	PRO A	190	20.168	73.057	-12 428	1 00	31.04
ATOM	1514	N	TYR A	191	20.220	74.051	-14.454	1 00	27.02
ATOM	1515	CA	TYR A	191	21.065	73.025	-15 054	1 00	25.82
ATOM	1516	CB	TYR A	191	20.612	72.611	-16 449	1.00	24.40
ATOM	1517	CG	TYR A	191	21.677	71.806	-17.164	1.00	23.94
ATOM	1518	CD1	TYR A	191	21.959	0.497	-16 779	1.00	24.85
ATOM	1519	CE1	TYR A	191	22.997	69.779	-17 370	1.00	26.57
ATOM	1520	CD2	TYR A	191	22.463	72.381	-18.169	1 00	24.25
ATOM	1521	CE2	TYR A	191	23.509	71.674	-18 764	1.00	22.72
ATOM	1522	CZ	TYR A	191	23.769	70.372	-18 359	1.00	27.36
ATOM	1523	OH	TYR A	191	24.791	69.655	-18 938	1.00	32.34
ATOM	1524	C	TYR A	191	22.406	73.737	-15.167	1.00	26.75
ATOM	1525	O	TYR A	191	22.477	74.848	-15.697	1.00	26.19
ATOM	1526	N	LEU A	192	23.453	73.131	-14.620	1.00	27.75
ATOM	1527	CA	LEU A	192	24.789	73.714	-14.662	1.00	30.44
ATOM	1528	C8	LEU A	192	25.134	74.378	-13.322	1.00	27.32
ATOM	1529	CG	LEU A	192	24.221	75.486	-12.789	1.00	24.54

ATOM	1530	CD1	LEU A	192	24 644	75.909	-11.386	1.00	20.65
ATOM	1531	CD2	LEU A	192	24.252	76 664	-13 738	1.00	21.14
ATOM	1532	C	LEU A	192	25.856	72 673	-15.013	1.00	34.74
ATOM	1533	O	LEU A	192	25.803	71 511	-14 586	1.00	33 09
ATOM	1534	N	ASP A	193	26.778	73 085	-15.867	1.00	36.86
ATOM	1535	CA	ASP A	193	27.877	72 250	-16.289	1.00	42.70
ATOM	1536	CB	ASP A	193	27.564	71 544	-17.600	1.00	48 25
ATOM	1537	CG	ASP A	193	28 732	70 728	-18.106	1 00	52.17
ATOM	1538	OD1	ASP A	193	29 125	70 928	-19.271	1 00	58 38
ATOM	1539	OD2	ASP A	193	29.266	69 897	-17 338	1.00	53.48
ATOM	1540	C	ASP A	193	29 032	73 196	-16 494	1.00	42.38
ATOM	1541	O	ASP A	193	29 061	73 951	-17.461	1 00	46.89
ATOM	1542	N	PRO A	194	29 994	73 178	-15 574	1 00	40.26
ATOM	1543	CD	PRO A	194	31 206	74.016	-15.565	1 00	40.20
ATOM	1544	CA	PRO A	194	29 956	72 294	-14.414	1 00	38.87
ATOM	1545	CB	PRO A	194	31.419	72.224	-14.018	1 00	39.32
ATOM	1546	CG	PRO A	194	31.863	73 644	-14.250	1 00	39.54
ATOM	1547	C	PRO A	194	29.082	72 863	-13 293	1.00	40.57
ATOM	1548	O	PRO A	194	28 773	74.065	-13.261	1 00	39 81
ATOM	1549	N	TYR A	195	28.667	71 976	-12.395	1 00	38.88
ATOM	1550	CA	TYR A	195	27.826	72 341	-11.269	1 00	35.95
ATOM	1551	CB	TYR A	195	26 869	71 187	-10.933	1.00	33.96
ATOM	1552	CG	TYR A	195	25.572	71.600	-10 255	1.00	33.27
ATOM	1553	CD1	TYR A	195	24.390	71.688	-10 984	1 00	32.32
ATOM	1554	CE1	TYR A	195	23 200	72 048	-10.381	1 00	31.47
ATOM	1555	CD2	TYR A	195	25 522	71.887	-8 889	1 00	29.66
ATOM	1556	CE2	TYR A	195	24 330	72.249	-8.276	1.00	27.38
ATOM	1557	CZ	TYR A	195	23.178	72 325	-9 030	1.00	27.54
ATOM	1558	OH	TYR A	195	21.996	72 665	-8.436	1.00	25.96
ATOM	1559	C	TYR A	195	28.726	72.624	-10.072	1.00	35.66
ATOM	1560	O	TYR A	195	29 616	71.832	-9 748	1.00	34 39
ATOM	1561	N	PRO A	196	28 505	73.762	-9.402	1.00	34.12
ATOM	1562	CD	PRO A	196	27 458	74.742	-9.730	1.00	32.84
ATOM	1563	CA	PRO A	196	29 270	74.183	-8.231	1.00	34.92
ATOM	1564	CB	PRO A	196	28.472	75.377	-7.735	1.00	35.33
ATOM	1565	CG	PRO A	196	27 915	75.951	-8.995	1.00	36 48
ATOM	1566	C	PRO A	196	29.276	73.076	-7.188	1.00	40.87
ATOM	1567	O	PRO A	196	28.257	72.808	-6.558	1.00	44.01
ATOM	1568	N	GLU A	197	30 418	72.425	-7.013	1.00	46.54
ATOM	1569	CA	GLU A	197	30.535	71.337	-6.048	1.00	49.40
ATOM	1570	CB	GLU A	197	31 992	70.896	-5 916	1.00	59.62
ATOM	1571	CG	GLU A	197	32 595	70.350	-7.211	1.00	74.74
ATOM	1572	CD	GLU A	197	34 093	70.061	-7 108	1.00	82 34
ATOM	1573	OE1	GLU A	197	34 807	70.797	-6 383	1.00	86 57
ATOM	1574	OE2	GLU A	197	34.558	69.100	-7 765	1.00	87 43
ATOM	1575	C	GLU A	197	30.007	71.757	-4.692	1.00	45 50
ATOM	1576	O	GLU A	197	29 395	70.972	-3 985	1.00	46.60
ATOM	1577	N	ALA A	198	30.216	73 018	-4 352	1.00	43.56
ATOM	1578	CA	ALA A	198	29.765	73.538	-3 072	1.00	42.05
ATOM	1579	CB	ALA A	198	30.214	74.968	-2 908	1.00	42.58
ATOM	1580	C	ALA A	198	28.264	73 443	-2.861	1.00	41.83
ATOM	1581	O	ALA A	198	27.805	73 315	-1.728	1.00	46.61
ATOM	1582	N	ALA A	199	27.501	73 501	-3.946	1.00	36 04
ATOM	1583	CA	ALA A	199	26.052	73 450	-3 852	1.00	32.51
ATOM	1584	CB	ALA A	199	25.430	74 173	-5.019	1.00	33.11
ATOM	1585	C	ALA A	199	25.512	72.044	-3.772	1.00	33 23
ATOM	1586	O	ALA A	199	24.307	71.837	-3.900	1.00	38 62
ATOM	1587	N	ILE A	200	26.397	71.075	-3.590	1.00	32 94
ATOM	1588	CA	ILE A	200	25 973	69.687	-3.508	1.00	34 13
ATOM	1589	CB	ILE A	200	26.565	68.846	-4.644	1.00	30.62
ATOM	1590	CG2	ILE A	200	26.086	67.409	-4.527	1.00	19 56
ATOM	1591	CG1	ILE A	200	26.154	69.451	-5.988	1.00	31 15
ATOM	1592	CD1	ILE A	200	27.065	69.109	-7.124	1.00	34.14
ATOM	1593	C	ILE A	200	26.353	69.073	-2.182	1.00	37.98
ATOM	1594	O	ILE A	200	27.525	68.817	-1.909	1.00	42.30
ATOM	1595	N	LYS A	201	25.343	68.844	-1.356	1.00	41.21
ATOM	1596	CA	LYS A	201	25.541	68.258	-0.045	1.00	42.08
ATOM	1597	CB	LYS A	201	24.485	68.776	0.935	1.00	44.17
ATOM	1598	CG	LYS A	201	24 592	70.275	1.203	1.00	47.76
ATOM	1599	CD	LYS A	201	23 219	70.918	1.218	1.00	52.10
ATOM	1600	CE	LYS A	201	23.302	72.423	1.021	1.00	52.22
ATOM	1601	NZ	LYS A	201	21.940	73.026	0.955	1.00	52.59
ATOM	1602	C	LYS A	201	25.443	66.761	-0.179	1.00	39.59

ATOM	1603	O	LYS	A	201	24.587	66.255	-0.886	1.00	42.27
ATOM	1604	N	THR	A	202	26.338	66.052	0.495	1.00	40.47
ATOM	1605	CA	THR	A	202	26.329	64.605	0.424	1.00	42.05
ATOM	1606	CB	THR	A	202	27.682	64.062	-0.114	1.00	38.96
ATOM	1607	OG1	THR	A	202	27.900	62.727	0.356	1.00	42.95
ATOM	1608	CG2	THR	A	202	28.838	64.970	0.276	1.00	40.84
ATOM	1609	C	THR	A	202	25.908	64.022	1.781	1.00	42.98
ATOM	1610	O	THR	A	202	26.553	64.247	2 809	1.00	47.33
ATOM	1611	N	ALA	A	203	24.750	63.369	1 785	1.00	41 07
ATOM	1612	CA	ALA	A	203	24 195	62.776	2.995	1.00	42 49
ATOM	1613	CB	ALA	A	203	22 824	62.179	2 713	1.00	36 69
ATOM	1614	C	ALA	A	203	25.110	61.705	3 525	1.00	44 40
ATOM	1615	O	ALA	A	203	25.924	61.159	2 787	1.00	45 26
ATOM	1616	N	ALA	A	204	24 920	61.348	4 788	1.00	47 23
ATOM	1617	CA	ALA	A	204	25.733	60.316	5 408	1.00	47 81
ATOM	1618	CB	ALA	A	204	25.266	60 089	6 817	1.00	48.23
ATOM	1619	C	ALA	A	204	25 701	59 000	4.615	1.00	48 73
ATOM	1620	O	ALA	A	204	26.680	58.252	4.581	1.00	51 77
ATOM	1621	N	ASP	A	205	24 574	58.725	3.970	1.00	45 72
ATOM	1622	CA	ASP	A	205	24.437	57 501	3 189	1.00	42 78
ATOM	1623	CB	ASP	A	205	22 984	56.989	2 221	1.00	47.36
ATOM	1624	CG	ASP	A	205	22.018	57.827	2 370	1.00	50 09
ATOM	1625	OD1	ASP	A	205	22.374	58 937	1 922	1 00	54.80
ATOM	1626	OD2	ASP	A	205	20.880	57 362	2.147	1.00	48 85
ATOM	1627	C	ASP	A	205	24 915	57 644	1 751	1 00	39 20
ATOM	1628	O	ASP	A	205	24 628	56 787	0 924	1 00	39.36
ATOM	1629	N	GLY	A	206	25 597	58 744	1.447	1 00	37.66
ATOM	1630	CA	GLY	A	206	26 100	58 968	0.097	1 00	36.43
ATOM	1631	C	GLY	A	206	25.238	59.669	-0.950	1.00	34 15
ATOM	1632	O	GLY	A	206	25 739	60.024	-2 017	1.00	31 94
ATOM	1633	N	THR	A	207	23 956	59 877	-0 679	1 00	29.49
ATOM	1634	CA	THR	A	207	23 109	60 538	-1.657	1 00	25.87
ATOM	1635	CB	THR	A	207	21.637	60 442	-1 260	1 00	27 03
ATOM	1636	OG1	THR	A	207	21.345	59.109	-0 824	1 00	29.78
ATOM	1637	CG2	THR	A	207	20 766	60 752	-2.447	1 00	28.36
ATOM	1638	C	THR	A	207	23 509	61.998	-1.837	1 00	25 47
ATOM	1639	O	THR	A	207	23 891	62 663	-0 881	1 00	27 07
ATOM	1640	N	LYS	A	208	23.481	62.478	-3.073	1 00	26 75
ATOM	1641	CA	LYS	A	208	23 828	63 866	-3.347	1 00	28 57
ATOM	1642	CB	LYS	A	208	24 323	64 035	-4 785	1 00	34 36
ATOM	1643	CG	LYS	A	208	25 565	63.216	-5 112	1.00	40 54
ATOM	1644	CD	LYS	A	208	26 734	63 592	-4 210	1.00	53.48
ATOM	1645	CE	LYS	A	208	27.937	62 669	-4 416	1 00	58 70
ATOM	1646	NZ	LYS	A	208	29 114	63.071	-3 586	1.00	62 46
ATOM	1647	C	LYS	A	208	22 540	64 626	-3 124	1.00	27 85
ATOM	1648	O	LYS	A	208	21 497	64 231	-3 638	1.00	29 27
ATOM	1649	N	LEU	A	209	22 620	65 743	-2.413	1 00	25 63
ATOM	1650	CA	LEU	A	209	21 442	66 518	-2.066	1 00	18 54
ATOM	1651	CB	LEU	A	209	21.149	66 348	-0 583	1 00	15 76
ATOM	1652	CG	LEU	A	209	21 027	64 949	-0 009	1.00	16 54
ATOM	1653	CD1	LEU	A	209	21 176	65.029	1.478	1.00	19.47
ATOM	1654	CD2	LEU	A	209	19 704	64.330	-0.393	1 00	14 83
ATOM	1655	C	LEU	A	209	21 570	67 997	-2.303	1.00	19 56
ATOM	1656	O	LEU	A	209	22 647	68 561	-2 184	1 00	20.20
ATOM	1657	N	SER	A	210	20 438	68 624	-2.591	1 00	20.72
ATOM	1658	CA	SER	A	210	20 359	70 064	-2.782	1 00	26 32
ATOM	1659	CA	SER	A	210	19 243	70 433	-3.770	1.00	26 58
ATOM	1660	OG	SER	A	210	19 611	70 186	-5.115	1.00	34 59
ATOM	1661	C	SER	A	210	20 000	70.625	-1 407	1 00	26 44
ATOM	1662	O	SER	A	210	20 466	71.694	-1.023	1.00	29 35
ATOM	1663	N	PHE	A	211	19 143	69.900	-0 683	1 00	27 04
ATOM	1664	CA	PHE	A	211	18 691	70.296	0 652	1 00	24.33
ATOM	1665	CB	PHE	A	211	17.306	70.938	0 603	1 00	25 32
ATOM	1666	CG	PHE	A	211	17.275	72.243	-0 123	1.00	27.69
ATOM	1667	CD1	PHE	A	211	16.682	72.341	-1 378	1 00	35 01
ATOM	1668	CD2	PHE	A	211	17.867	73.370	0 426	1 00	31.73
ATOM	1669	CE1	PHE	A	211	16.681	73.547	-2 082	1 00	35.58
ATOM	1670	CE2	PHE	A	211	17.875	74.586	-0 269	1 00	34.04
ATOM	1671	CZ	PHE	A	211	17.281	74.672	-1.525	1.00	36.38
ATOM	1672	C	PHE	A	211	18.670	69.116	1.611	1.00	24.35
ATOM	1673	O	PHE	A	211	18.062	68.076	1.339	1.00	21.15
ATOM	1674	N	GLU	A	212	19.354	69.304	2.732	1.00	25.04
ATOM	1675	CA	GLU	A	212	19.485	68.311	3.777	1.00	26.00

ATOM	1676	CB	GLU A	212	20 580	68.763	4.742	1.00	31.89
ATOM	1677	CG	GLU A	212	21 004	67.726	5.770	1.00	52.30
ATOM	1678	CD	GLU A	212	21.606	66.472	5.145	1 00	60 61
ATOM	1679	OE1	GLU A	212	20.903	65.434	5.092	1 00	59 97
ATOM	1680	OE2	GLU A	212	22 786	66.527	4.718	1.00	67 14
ATOM	1681	C	GLU A	212	18 158	68.100	4.500	1.00	24.80
ATOM	1682	O	GLU A	212	17 243	68.918	4.392	1.00	22 54
ATOM	1683	N	TRP A	213	18 059	66.997	5.234	1 00	26 64
ATOM	1684	CA	TRP A	213	16.846	66.653	5.963	1 00	28 18
ATOM	1685	CB	TRP A	213	17.062	65.393	6.811	1 00	27 08
ATOM	1686	CG	TRP A	213	17.942	65.589	7 993	1 00	31.90
ATOM	1687	CD2	TRP A	213	17.541	66.016	9 295	1.00	34.81
ATOM	1688	CE2	TRP A	213	18.702	66.070	10 093	1.00	39.48
ATOM	1689	CE3	TRP A	213	16 310	66.353	9 867	1 00	35.14
ATOM	1690	CD1	TRP A	213	19.291	65.406	8.051	1.00	34 70
ATOM	1691	NE1	TRP A	213	19.759	65 698	9 306	1.00	38 91
ATOM	1692	CZ2	TRP A	213	18.671	66 456	11 436	1.00	39.22
ATOM	1693	CZ3	TRP A	213	16 278	66 736	11 198	1.00	36.20
ATOM	1694	CH2	TRP A	213	17.452	66 780	11 969	1.00	39 04
ATOM	1695	C	TRP A	213	16.312	67.780	6 840	1.00	27 32
ATOM	1696	O	TRP A	213	17.074	68 601	7 341	1.00	26 78
ATOM	1697	N	HIS A	214	14.994	67 785	7 033	1.00	25 99
ATOM	1698	CA	HIS A	214	14.312	68.785	9 843	1:00	21.26
ATOM	1699	CB	HIS A	214	14.498	70 170	7.229	1.00	24 00
ATOM	1700	CG	HIS A	214	14.011	70.268	5 815	1.00	26 31
ATOM	1701	CD2	HIS A	214	12.986	70.964	5.265	1.00	20 40
ATOM	1702	ND1	HIS A	214	14.604	69.575	4.782	1.00	24.70
ATOM	1703	CE1	HIS A	214	13.966	69 840	3.657	1.00	19.84
ATOM	1704	NE2	HIS A	214	12.983	70.682	3.921	1.00	19.56
ATOM	1705	C	HIS A	214	12.824	68.508	7 915	1.00	20 75
ATOM	1706	O	HIS A	214	12.295	67.628	7.230	1.00	22.27
ATOM	1707	N	GLU A	215	12.153	69 316	8.718	1.00	21.29
ATOM	1708	Q	GLU A	215	10.710	69 258	8.888	1.00	25.72
ATOM	1709	CB	GLU A	215	10.347	68.937	10.341	1.00	27.88
ATOM	1710	CG	GLU A	215	11.325	69.505	11.344	1.00	44.01
ATOM	1711	CD	GLU A	215	10.962	69.188	12.773	1.00	49.99
ATOM	1712	OE1	GLU A	215	10.532	68 043	13.040	1.00	48.65
ATOM	1713	OE2	GLU A	215	11.118	70 089	13.628	1.00	56.84
ATOM	1714	C	GLU A	215	10.320	70.676	8.504	1.00	23.84
ATOM	1715	O	GLU A	215	11.116	71 595	8.672	1.00	24.88
ATOM	1716	N	ASP A	216	9.136	70 858	7.935	1.00	22.73
ATOM	1717	CA	ASP A	216	8.732	72.187	7.492	1.00	22.94
ATOM	1718	CB	ASP A	216	7.636	72.112	6.407	1.00	27.97
ATOM	1719	CG	ASP A	216	8.082	71.398	5.135	1.00	27.71
ATOM	1720	OD1	ASP A	216	9.304	71.232	4.918	1.00	31.88
ATOM	1721	OD2	ASP A	216	7.185	71.015	4.344	1.00	26.49
ATOM	1722	C	ASP A	216	8 230	73.096	8.596	1.00	19.73
ATOM	1723	O	ASP A	216	7 680	72.652	9.594	1.00	23.16
ATOM	1724	N	VAL A	217	8.433	74 384	8.398	1.00	16.59
ATOM	1725	CA	VAL A	217	7 945	75 376	9.312	1.00	18.55
ATOM	1726	CB	VAL A	217	8.907	76.564	9.424	1.00	16.49
ATOM	1727	CG1	VAL A	217	8.265	77 687	10.235	1.00	10.45
ATOM	1728	CG2	VAL A	217	10.179	76.123	10.088	1.00	11.70
ATOM	1729	C	VAL A	217	6.652	75 819	8.633	1.00	23.10
ATOM	1730	O	VAL A	217	6.667	76 674	7.729	1.00	21.60
ATOM	1731	N	SER A	218	5.562	75 142	8.990	1.00	25.06
ATOM	1732	CA	SER A	218	4.233	75 433	8.452	1.00	24.44
ATOM	1733	CB	SER A	218	4.183	75 110	6.954	1.00	23.25
ATOM	1734	OG	SER A	218	4.109	73.706	6.717	1.00	16 35
ATOM	1735	C	SER A	218	3.190	74.585	9.178	1.00	23.44
ATOM	1736	O	SER A	218	3.541	73.734	9.996	1.00	23 65
ATOM	1737	N	LEU A	219	1.913	74.865	8.932	1.00	21.85
ATOM	1738	CA	LEU A	219	0.847	74.064	9.518	1.00	22 52
ATOM	1739	CB	LEU A	219	-0.493	74.797	9.483	1.00	22 11
ATOM	1740	CG	LEU A	219	-1.687	73.960	9.955	1.00	18.98
ATOM	1741	CD1	LEU A	219	-2 427	73.419	11.330	1.00	17 47
ATOM	1742	CD2	LEU A	219	-2 933	74.804	9 956	1.00	19 86
ATOM	1743	C	LEU A	219	0 822	72.817	8 633	1.00	24 74
ATOM	1744	O	LEU A	219	0 870	71.697	9 128	1.00	26 48
ATOM	1745	N	ILE A	220	0 760	73.030	7 318	1.00	24 79
ATOM	1746	CA	ILE A	220	0 821	71.960	6 309	1.00	22 56
ATOM	1747	CB	ILE A	220	-0 563	71.393	5.860	1.00	21 63
ATOM	1748	CG2	ILE A	220	-1 335	70.840	7.040	1.00	20.63

ATOM	1749	CG1	ILE A	220	-1.380	72.443	5.109	1.00	22.42
ATOM	1750	CD1	ILE A	220	-2.505	71.841	4.297	1.00	18.13
ATOM	1751	C	ILE A	220	1.501	72.600	5.099	1.00	18.56
ATOM	1752	O	ILE A	220	1.496	73.825	4.970	1.00	17.45
ATOM	1753	N	THR A	221	2.141	71.793	4.263	1.00	17.74
ATOM	1754	CA	THR A	221	2.802	72.295	3.069	1.00	14.91
ATOM	1755	CB	THR A	221	4.287	71.939	3.032	1.00	15.95
ATOM	1756	OG1	THR A	221	4.937	72.557	4.146	1.00	18.73
ATOM	1757	CG2	THR A	221	4.928	72.469	1.773	1.00	10.41
ATOM	1758	C	THR A	221	2.066	71 651	1.916	1.00	16.30
ATOM	1759	O	THR A	221	1.711	70 477	1.983	1.00	18.87
ATOM	1760	N	VAL A	222	1.729	72 477	0.933	1.00	16.62
ATOM	1761	CA	VAL A	222	0.992	72 088	-0.261	1.00	17.81
ATOM	1762	CB	VAL A	222	-0.332	72.880	-0.310	1.00	22.05
ATOM	1763	CG1	VAL A	222	-1.046	72.671	-1.630	1.00	25.61
ATOM	1764	CG2	VAL A	222	-1.221	72 446	0.854	1.00	24.18
ATOM	1765	C	VAL A	222	1.890	72 404	-1.464	1.00	17.84
ATOM	1766	O	VAL A	222	1.990	73.557	-1.895	1.00	18.42
ATOM	1767	N	LEU A	223	2.525	71.359	-1.995	1.00	14.96
ATOM	1768	CA	LEU A	223	3.495	72.469	-3.080	1.00	15.97
ATOM	1769	CB	LEU A	223	4.779	70 761	-2.647	1.00	8 17
ATOM	1770	CG	LEU A	223	5.836	70 407	-3.680	1.00	9 19
ATOM	1771	CD1	LEU A	223	6.771	71 557	-3.882	1.00	9 69
ATOM	1772	CD2	LEU A	223	6.605	69 205	-3 192	1.00	12 71
ATOM	1773	C	LEU A	223	3.146	70.951	-4 462	1.00	20 09
ATOM	1774	O	LEU A	223	2 623	69 846	-4 608	1.00	24 25
ATOM	1775	N	TYR A	224	3.453	71 757	-5 476	1.00	23 92
ATOM	1776	CA	TYR A	224	3.283	71 340	-6 862	1.00	22.47
ATOM	1777	CB	TYR A	224	2.425	72 269	-7 711	1.00	25.33
ATOM	1778	CG	TYR A	224	2.258	71.701	-9 110	1.00	24.10
ATOM	1779	CD1	TYR A	224	1.592	70 488	-9.311	1.00	22 12
ATOM	1780	CE1	TYR A	224	1.534	69 893	-10 560	1.00	25 03
ATOM	1781	CD2	TYR A	224	2.860	72 311	-10.212	1.00	23 73
ATOM	1782	CE2	TYR A	224	2 811	71.720	-11.475	1.00	27.76
ATOM	1783	CZ	TYR A	224	2 146	70 505	-11.643	1.00	29 83
ATOM	1784	OH	TYR A	224	2 112	69 895	-12.884	1.00	31 58
ATOM	1785	C	TYR A	224	4 680	71.314	-7 451	1.00	25 24
ATOM	1786	O	TYR A	224	5 424	72 301	-7 392	1 00	27 50
ATOM	1787	N	GLN A	225	5.014	70.193	-8.060	1 00	23.63
ATOM	1788	CA	GLN A	225	6 327	70 006	-8.639	1 00	25 73
ATOM	1789	Q	GLN A	225	7 184	69.294	-7 609	1 00	23.37
ATOM	1790	CG	GLN A	225	8.614	69 292	-7 891	1 00	25.23
ATOM	1791	CD	GLN A	225	9 378	68 781	-6 720	1 00	30 69
ATOM	1792	OE1	GLN A	225	10 264	69 461	-6 203	1 00	37 77
ATOM	1793	NE2	GLN A	225	9 042	67 578	-6 278	1 00	29 82
ATOM	1794	C	GLN A	225	6 105	69.126	-9 858	1 00	27 45
ATOM	1795	O	GLN A	225	5 503	68 056	-9 759	1 00	27 59
ATOM	1796	N	SER A	226	6.601	69 552	-11.007	1 00	27.34
ATOM	1797	CA	SER A	226	6 358	68.779	-12.210	1 00	28 99
ATOM	1798	CB	SER A	226	5.501	69.605	-13 152	1 00	28 18
ATOM	1799	OG	SER A	226	5 052	68 829	-14.229	1 00	40.16
ATOM	1800	C	SER A	226	7 599	68.311	-12.943	1.00	31 56
ATOM	1801	O	SER A	226	8 570	69.055	-13 087	1 00	32 05
ATOM	1802	N	ASN A	227	7 571	67 055	-13 370	1 00	30.89
ATOM	1803	CA	ASN A	227	8 667	66 471	-14.133	1 00	29 18
ATOM	1804	CB	ASN A	227	8 878	67.285	-15 417	1 00	28.72
ATOM	1805	CG	ASN A	227	9 511	66 482	-16.528	1 00	27 74
ATOM	1806	OD1	ASN A	227	9.130	65 341	-16.779	1 00	28 75
ATOM	1807	ND2	ASN A	227	10 454	67 089	-17.229	1 00	27 94
ATOM	1808	C	ASN A	227	9 990	66 328	-13.380	1 00	28.97
ATOM	1809	O	ASN A	227	11.052	66 517	-13.960	1 00	30 10
ATOM	1810	N	VAL A	228	9 929	66 006	-12.091	1 00	29 20
ATOM	1811	CA	VAL A	228	11.135	65 809	-11.291	1 00	27.27
ATOM	1812	CB	VAL A	228	11.599	67 058	-10 497	1.00	26 29
ATOM	1813	CG1	VAL A	228	13 083	67 241	-10 649	1.00	23 43
ATOM	1814	CG2	VAL A	228	10 827	68 292	-10 859	1.00	25 97
ATOM	1815	C	VAL A	228	10 799	64.826	-10 206	1.00	31 99
ATOM	1816	O	VAL A	228	9 651	64.760	-9 758	1.00	35 97
ATOM	1817	N	GLN A	229	11 822	64.110	-9 753	1.00	34 06
ATOM	1818	CA	GLN A	229	11 715	63.153	-8 658	1.00	33 36
ATOM	1819	CB	GLN A	229	11.795	61.734	-9.176	1.00	37 53
ATOM	1820	CG	GLN A	229	11.559	60.666	-8 148	1.00	42 23
ATOM	1821	CD	GLN A	229	11.207	59.368	-8.833	1.00	55.26

ATOM	1822	OE1	GLN	A	229	10.110	59.222	-9.392	1.00	58.46
ATOM	1823	NE2	GLN	A	229	12 155	58.436	-8 857	1.00	59.25
ATOM	1824	C	GLN	A	229	12 935	63.474	-7.814	1.00	34.22
ATOM	1825	O	GLN	A	229	14.044	63.042	-8 124	1.00	34.78
ATOM	1826	N	ASN	A	230	12 733	64.293	-6 784	1.00	34.28
ATOM	1827	CA	ASN	A	230	13.827	64.732	-5 917	1.00	32 42
ATOM	1828	C8	ASN	A	230	14 171	66.199	-6 226	1 00	27.53
ATOM	1829	CG	ASN	A	230	12 974	67.136	-6 068	1.00	21.96
ATOM	1830	OD1	ASN	A	230	11 933	66.751	-5.545	1 00	24.46
ATOM	1831	ND2	ASN	A	230	13 118	68.361	-6 541	1.00	19.87
ATOM	1832	C	ASN	A	230	13.575	64.587	-4.419	1 00	31.95
ATOM	1833	O	ASN	A	230	14 476	64.808	-3 622	1.00	30.47
ATOM	1834	N	LEU	A	231	12.356	64.231	-4.034	1.00	31.28
ATOM	1835	CA	LEU	A	231	12.018	64.092	-2 626	1.00	27.98
ATOM	1836	CB	LEU	A	231	10.551	64.431	-2 408	1.00	24.65
ATOM	1837	CG	LEU	A	231	10.254	65.884	-2.135	1 00	21.29
ATOM	1838	CD1	LEU	A	231	8.807	65.985	-1.745	1 00	24 61
ATOM	1839	CD2	LEU	A	231	11.116	66.349	-0.993	1 00	23.04
ATOM	1840	C	LEU	A	231	12 276	62.719	-2.040	1.00	30 04
ATOM	1841	O	LEU	A	231	12.145	61.706	-2.725	1 00	34 74
ATOM	1842	N	GLN	A	232	12 615	62.693	-0.754	1 00	30.14
ATOM	1843	CA	GLN	A	232	12.834	61.418	-0.034	1 00	26 30
ATOM	1844	CB	GLN	A	232	14 314	61.087	0 000	1 00	25 18
ATOM	1845	CG	GLN	A	232	14 877	60.607	-1.315	1 00	24 42
ATOM	1846	CD	GLN	A	232	16.251	59 976	-1 163	1 00	28.50
ATOM	1847	OE1	GLN	A	232	17 149	60 543	-0 538	1.00	29.12
ATOM	1848	NE2	GLN	A	232	16.420	58.794	-1 736	1 00	27 79
ATOM	1849	C	GLN	A	232	12.313	61.614	1 392	1.00	27 21
ATOM	1850	O	GLN	A	232	12 538	62.656	2.015	1.00	29 07
ATOM	1851	N	VAL	A	233	11 581	60.618	1 888	1.00	25.56
ATOM	1852	CA	VAL	A	233	11.047	60.659	3.250	1.00	23.90
ATOM	1853	CB	VAL	A	233	9.588	60.295	3.354	1.00	26.06
ATOM	1854	CG1	VAL	A	233	8 862	61.027	4.382	1.00	28.07
ATOM	1855	CG2	VAL	A	233	8.911	60.178	2 027	1 00	25.39
ATOM	1856	C	VAL	A	233	11.779	59.644	4.101	1 00	27.04
ATOM	1857	O	VAL	A	233	12 024	58.519	3.662	1.00	27.08
ATOM	1858	N	GLU	A	234	12.090	60.015	5.331	1.00	27.08
ATOM	1859	CA	GLU	A	234	12 744	59 089	6.226	1.00	28.63
ATOM	1860	CB	GLU	A	234	13.512	59 848	7.289	1.00	28 65
ATOM	1861	CG	GLU	A	234	14.044	58 977	8.400	1.00	33 81
ATOM	1862	CD	GLU	A	234	14.652	59 788	9.509	1.00	37.83
ATOM	1863	OE1	GLU	A	234	15 893	59.870	9.558	1.00	46.49
ATOM	1864	OE2	GLU	A	234	13.894	60.356	10.323	1 00	41.82
ATOM	1865	C	GLU	A	234	12.637	58.292	6.881	1 00	32.99
ATOM	1866	O	GLU	A	234	10 761	58 861	7.526	1.00	36.86
ATOM	1867	N	THR	A	235	11 619	56 990	6.654	1 00	39 05
ATOM	1868	CA	THR	A	235	10 603	56.144	7.264	1 00	43.64
ATOM	1869	CB	THR	A	235	9 789	55.370	6.196	1 00	47 64
ATOM	1870	OG1	THR	A	235	10.663	54.518	5.443	1.00	48 96
ATOM	1871	CG2	THR	A	235	9.077	56.340	5.245	1 00	49.04
ATOM	1872	C	THR	A	235	11.310	55.161	8.186	1.00	45.27
ATOM	1873	O	THR	A	235	12.533	55.204	8.330	1 00	46.15
ATOM	1874	N	ALA	A	236	10.549	54.266	8.802	1 00	48.85
ATOM	1875	CA	ALA	A	236	11.131	53.271	9.697	1.00	51 37
ATOM	1876	CB	ALA	A	236	10.035	52.506	10.416	1.00	52.57
ATOM	1877	C	ALA	A	236	12.049	52.307	8.944	1 00	51.92
ATOM	1878	O	ALA	A	236	12.709	51.464	9.547	1.00	56.47
ATOM	1879	N	ALA	A	237	12.044	52.402	7.620	1.00	50 60
ATOM	1880	CA	ALA	A	237	12.886	51.558	6.786	1.00	50.28
ATOM	1881	CB	ALA	A	237	12.044	50.870	5.720	1 00	45.48
ATOM	1882	C	ALA	A	237	13.952	52.421	6.126	1.00	51.53
ATOM	1883	O	ALA	A	237	14.591	51.992	5.156	1.00	53.02
ATOM	1884	N	GLY	A	238	14.159	53.620	6.672	1.00	49.22
ATOM	1885	CA	GLY	A	238	15.129	54.542	6.108	1.00	47.88
ATOM	1886	C	GLY	A	238	14.493	55.410	5.029	1.00	46.36
ATOM	1887	O	GLY	A	238	13.275	55.377	4.837	1.00	45.44
ATOM	1888	N	TYR	A	239	15.305	56.193	4.325	1.00	43.94
ATOM	1889	CA	TYR	A	239	14.795	57.077	3 282	1.00	42.31
ATOM	1890	CB	TYR	A	239	15.860	58.079	2 862	1.00	34.38
ATOM	1891	CG	TYR	A	239	16.054	59.203	3 846	1.00	31.86
ATOM	1892	CD1	TYR	A	239	16.902	59.064	4 943	1.00	29.03
ATOM	1893	CE1	TYR	A	239	17.115	60.129	5 825	1.00	30.21
ATOM	1894	CD2	TYR	A	239	15.416	60.427	3 659	1.00	31.58

ATOM	1895	CE2	TYR A	239	15.618	61.491	4.536	1.00	27.77
ATOM	1896	CZ	TYR A	239	16.467	61.337	5.609	1.00	28.27
ATOM	1897	OH	TYR A	239	16.670	62.396	6.459	1.00	30.28
ATOM	1898	C	TYR A	239	14.282	56.345	2.053	1.00	44.26
ATOM	1899	O	TYR A	239	14.958	55.464	1.519	1.00	50.07
ATOM	1900	N	GLN A	240	13.089	56.730	1.605	1.00	42.95
ATOM	1901	CA	GLN A	240	12 457	56.135	0.434	1.00	37.56
ATOM	1902	CB	GLN A	240	11.227	55.338	0.829	1.00	37.90
ATOM	1903	CG	GLN A	240	11 492	54.283	1.867	1.00	39.00
ATOM	1904	CD	GLN A	240	10 259	53.503	2.178	1.00	41 54
ATOM	1905	OE1	GLN A	240	9 361	53.975	2.876	1.00	42 44
ATOM	1906	NE2	GLN A	240	10.192	52.303	1.655	1.00	43 71
ATOM	1907	C	GLN A	240	12 036	57.238	-0.493	1.00	35 12
ATOM	1908	O	GLN A	240	11 637	58 310	-0.049	1 00	37 16
ATOM	1909	N	ASP A	241	12 106	56 963	-1.786	1 00	37 65
ATOM	1910	CA	ASP A	241	11 757	57 937	-2.807	1.00	33.97
ATOM	1911	CB	ASP A	241	12 294	57 477	-4.157	1.00	36 71
ATOM	**1912**	**CG**	**ASP A**	**241**	**13 768**	**57 725**	**-4.305**	**1.00**	**40 53**
ATOM	1913	OD1	ASP A	241	14 501	56 767	-4.626	1.00	48 07
ATOM	1914	OD2	ASP A	241	14.193	58 883	-4.102	1 00	43.60
ATOM	191S	C	ASP A	241	10 273	58.187	-2.937	1 00	31.87
ATOM	1916	O	ASP A	241	9 473	57 290	-2.715	1 00	33 89
ATOM	1917	N	ILE A	242	9 910	59 420	-3.270	1 00	29.50
ATOM	1918	CA	ILE A	242	8 516	59 776	-3 491	1.00	29 59
ATOM	1919	CB	ILE A	242	8 122	61.110	-2 793	1 00	25.82
ATOM	1920	CG2	ILE A	242	6.718	61 540	-3.205	1 00	21 57
ATOM	1921	CG1	ILE A	242	8 142	60 940	-1.275	1.00	22 34
ATOM	1922	CD1	ILE A	242	7 931	62.219	-0.529	1 00	19.47
ATOM	1923	C	ILE A	242	8 324	59 899	-5.002	1.00	32 14
ATOM	1924	O	ILE-A	242	9 039	60 631	-5.680	1 00	34.26
ATOM	1925	N	GLU A	243	7.364	59 139	-5.528	1.00	32.42
ATOM	1926	CA	GLU A	243	7 051	59 161	-6 950	1.00	35.87
ATOM	1927	CB	GLU A	243	5 998	58 103	-7.257	1 00	45.32
ATOM	1928	CG	GLU A	243	4 620	58.422	-6 675	1 00	58.52
ATOM	1929	CD	GLU A	243	3 584	57 359	-6 970	1 00	67.74
ATOM	1930	OE1	GLU A	243	2.679	57 157	-6 126	1 00	72 36
ATOM	1931	OE2	GLU A	243	3 669	56 730	-8 048	1 00	73 67
ATOM	1932	C	GLU A	243	6 494	60.520	-7 361	1.00	34 26
ATOM	1933	O	GLU A	243	5 794	61 170	-6 587	1.00	34.70
ATOM	1934	N	ALA A	244	6 796	60.940	-8.582	1 00	37.24
ATOM	1935	CA	ALA A	244	6.299	62.211	-9 106	1 00	36 70
ATOM	1936	CB	ALA A	244	7.187	62 704	-10 237	1 00	30 95
ATOM	1937	C	ALA A	244	4 870	62.045	-9 607	1 00	38 29
ATOM	1938	O	ALA A	244	4 401	60 919	-9 809	1 00	39 49
ATOM	1939	N	ASP A	245	4.184	63.168	-9 810	1 00	38.94
ATOM	1940	CA	ASP A	245	2 809	63 171	-10 302	1 00	36.20
ATOM	1941	CB	ASP A	245	1 849	62 683	-9.217	1 00	35 69
ATOM	1942	CG	ASP A	245	0 436	62.479	-9.730	1 00	39.12
ATOM	1943	OD1	ASP A	245	-0 090	63 350	-10 446	1 00	38.32
ATOM	1944	OD2	ASP A	245	-0.162	61.440	-9 406	1 00	44.34
ATOM	1945	C	ASP A	245	2 423	64 579	-10.720	1 00	36.64
ATOM	1946	O	ASP A	245	1 881	65 338	-9.920	1.00	40 34
ATOM	1947	N	ASP A	246	2 624	64.906	-11 989	1 00	36 70
ATOM	1948	CA	ASP A	246	2 288	66.242	-12.464	1 00	42.59
ATOM	1949	CB	ASP A	246	2 956	66 546	-13 815	1 00	52 74
ATOM	1950	CG	ASP A	246	2 651	65.508	-14 899	1 00	62 16
ATOM	1951	OD1	ASP A	246	3 484	65 398	-15.834	1 00	67 79
ATOM	1952	OD2	ASP A	246	1 600	64 822	-14 836	1 00	61 80
ATOM	1953	C	ASP A	246	0 818	66.649	-12.495	1 00	39 27
ATOM	1954	O	ASP A	246	0 485	67 699	-13 042	1 00	39.09
ATOM	1955	N	THR A	247	-0 058	65 849	-11 897	1 00	37 20
ATOM	1956	CA	THR A	247	-1.475	66.182	-11 876	1 00	37.88
ATOM	1957	CB	THR A	247	-2 345	65 074	-12 545	1.00	41.31
ATOM	1958	OG1	THR A	247	-2.370	63 901	-11 719	1.00	44 54
ATOM	1959	CG2	THR A	247	-1 770	64 688	-13 903	1.00	42 77
ATOM	1960	C	THR A	247	-1 990	66 436	-10 452	1.00	37 11
ATOM	1961	O	THR A	247	-3 109	66 933	-10.263	1.00	35 84
ATOM	1962	N	GLY A	248	-1 162	66.136	-9 453	1.00	33 34
ATOM	1963	CA	GLY A	248	-1 580	66 320	-8.076	1.00	29.08
ATOM	1964	C	GLY A	248	-0.704	67 236	-7.251	1.00	26.86
ATOM	1965	O	GLY A	248	0.338	67 693	-7.709	1.00	29.61
ATOM	1966	N	TYR A	249	-1.168	67.553	-6.052	1.00	24.24
ATOM	1967	CA	TYR A	249	-0.432	68.401	-5.128	1.00	22.26

ATOM	1968	CB	TYR A	249	-1.319	69.512	-4.571	1.00	17.04
ATOM	1969	CG	TYR A	249	-1.337	70.775	-5.395	1.00	19.97
ATOM	1970	CD1	TYR A	249	-2.159	70.896	-6 505	1.00	21.32
ATOM	1971	CE1	TYR A	249	-2.194	72.078	-7 247	1.00	22 14
ATOM	1972	CD2	TYR A	249	-0.545	71.866	-5 045	1.00	17 14
ATOM	1973	CE2	TYR A	249	-0 575	73.041	-5.777	1.00	18 05
ATOM	1974	CZ	TYR A	249	-1 398	73 140	-6 876	1 00	18 13
ATOM	1975	OH	TYR A	249	-1 412	74 302	-7 612	1.00	23.74
ATOM	1976	C	TYR A	249	0.037	67 520	-3 982	1.00	24.44
ATOM	1977	O	TYR A	249	-0.766	66 820	-3.363	1.00	25.35
ATOM	1978	N	LEU A	250	1.344	67 505	-3.745	1 00	21.09
ATOM	1979	CA	LEU A	250	1.908	66 720	-2.664	1 00	19.72
ATOM	1980	CB	LEU A	250	3.397	66 484	-2 914	1.00	11.66
ATOM	1981	CG	LEU A	250	4 092	65 533	-1 946	1.00	13.51
ATOM	1982	CD1	LEU A	250	3 460	64 158	-1 998	1.00	9 39
ATOM	1983	CD2	LEU A	250	5.536	65.450	-2 310	1.00	16 26
ATOM	1984	C	LEU A	250	1.683	67 475	-1.349	1 00	24.50
ATOM	1985	O	LEU A	250	2.160	68.606	-1.176	1.00	23.74
ATOM	1986	N	ILE A	251	0.953	66 847	-0.432	1.00	25.00
ATOM	1987	CA	ILE A	251	0.651	67 447	0 866	1 00	23.54
ATOM	1988	CB	ILE A	251	-0.876	67 411	1 138	1 00	21.64
ATOM	1989	CG2	ILE A	251	-1.257	68.522	2.121	1.00	20.73
ATOM	1990	CG1	ILE A	251	-2.670	67.562	-0.169	1.00	18.11
ATOM	1991	CD1	ILE A	251	-2.594	68 929	-0.792	1.00	15 82
ATOM	1992	C	ILE A	251	1 376	66.775	2.071	1.00	25.96
ATOM	1993	O	ILE A	251	1.478	65 545	2 148	1 00	22.81
ATOM	1994	N	ASN A	252	1.919	67 590	2.979	1.00	27.93
ATOM	1995	CA	ASN A	252	2.583	67.097	4 190	1 00	23 28
ATOM	1996	CB	ASN A	252	4 067	66.731	3.969	1 00	19 24
ATOM	1997	CG	ASN A	252	4.943	67 922	3.669	1.00	15 95
ATOM	1998	OD1	ASN A	252	5 210	68 225	2.521	1.00	27 71
ATOM	1999	ND2	ASN A	252	5 482	68 544	4.698	1.00	12.20
ATOM	2000	C	ASN A	252	2 417	68.107	5.321	1.00	26.77
ATOM	2001	O	ASN A	252	2.046	69.258	5 079	1.00	26.57
ATOM	2002	N	CYS A	253	2 621	67.649	6 555	1.00	26 39
ATOM	2003	CA	CYS A	253	2.484	68 488	7 744	1.00	23 80
ATOM	2004	CB	CYS A	253	2 069	67.638	8 950	1.00	26 15
ATOM	2005	SG	CYS A	253	0 326	67.176	9.038	1.00	32.10
ATOM	2006	C	CYS A	253	3 758	69.222	8.107	1.00	20.68
ATOM	2007	O	CYS A	253	4 853	68.766	7.810	1.00	23.52
ATOM	2008	N	GLY A	254	3 601	70.371	8 740	1.00	21.10
ATOM	2009	CA	GLY A	254	4.740	71.143	9.183	1.00	21 44
ATOM	2010	C	GLY A	254	4.870	70.886	10.669	1.00	19.86
ATOM	2011	O	GLY A	254	4.062	70.173	11.245	1.00	17.78
ATOM	2012	N	SER A	255	5.839	71.492	11.325	1.00	21.03
ATOM	2013	CA	SER A	255	5.996	71.237	12.737	1.00	20.86
ATOM	2014	CB	SER A	255	7.348	71.742	13.225	1.00	16.65
ATOM	2015	OG	SER A	255	7.529	73.096	12.870	1.00	24.84
ATOM	2016	C	SER A	255	4.862	71.800	13.592	1.00	25.80
ATOM	2017	O	SER A	255	4.635	71.316	14.702	1.00	32.81
ATOM	2018	N	TYR A	256	4.132	72.800	13.103	1.00	23.31
ATOM	2019	CA	TYR A	256	3.048	73.337	13.916	1.00	22.05
ATOM	2020	CB	TYR A	256	2.453	74.597	13.320	1.00	18.59
ATOM	2021	CG	TYR A	256	1.600	75.359	14.313	1.00	18.81
ATOM	2022	CD1	TYR A	256	2.181	76.147	15.301	1.00	14.81
ATOM	2023	CE1	TYR A	256	1.399	76.878	16.198	1.00	18.34
ATOM	2024	CD2	TYR A	256	0.213	75.302	14.253	1.00	22.82
ATOM	2025	CE2	TYR A	256	-0.586	76.029	15.151	1.00	22.41
ATOM	2026	CZ	TYR A	256	0.015	76.812	16.122	1.00	22.48
ATOM	2027	OH	TYR A	256	-0.777	77.531	16.994	1.00	27.35
ATOM	2028	C	TYR A	256	1.946	72.303	14.160	1.00	25.24
ATOM	2029	O	TYR A	256	1.377	72.250	15.249	1.00	30.73
ATOM	2030	N	MET A	257	1.645	71.490	13.152	1.00	25.21
ATOM	2031	CA	MET A	257	0.633	70.443	13.281	1.00	25.59
ATOM	2032	CB	MET A	257	0.422	69.749	11.930	1.00	23.11
ATOM	2033	CG	MET A	257	-0.631	68.646	11.889	1.00	23.77
ATOM	2034	SD	MET A	257	-2.303	69.226	12.196	1.00	29.13
ATOM	2035	CE	MET A	257	-2.926	69 464	10.571	1.00	21.14
ATOM	2036	C	MET A	257	1.118	69 444	14.338	1.00	29.65
ATOM	2037	O	MET A	257	0.348	68 996	15.182	1.00	33.68
ATOM	2038	N	ALA A	258	2.410	69.139	14.324	1.00	30.20
ATOM	2039	CA	ALA A	258	2.975	68.207	15.294	1.00	29.21
ATOM	2040	CB	ALA A	258	4.437	67.918	14.962	1.00	26.53

ATOM	2041	C	ALA	A	258	2.843	68.740	16 721	1.00	29.82
ATOM	2042	O	ALA	A	258	2.486	67.999	17 635	1.00	30.07
ATOM	2043	N	HIS	A	259	3.130	70.023	16 912	1.00	29 81
ATOM	2044	CA	HIS	A	259	3 022	70.635	18 231	1.00	30 03
ATOM	2045	CB	HIS	A	259	3 560	72.062	18 197	1.00	29 44
ATOM	2046	CG	HIS	A	259	3 279	72.846	19.441	1.00	36 67
ATOM	2047	CD2	HIS	A	259	3 972	72 971	20.600	1 00	35 37
ATOM	2048	ND1	HIS	A	259	2.174	73 662	19 572	1 00	39 99
ATOM	2049	CE1	HIS	A	259	2 201	74 255	20.750	1 00	40 29
ATOM	2050	NE2	HIS	A	259	3.284	73 854	21.397	1 00	33 91
ATOM	2051	C	HIS	A	259	1.571	70 645	18 703	1.00	32 65
ATOM	2052	O	HIS	A	259	1.295	70 499	19 884	1 00	37.28
ATOM	2053	N	LEU	A	260	0.650	70 862	17.778	1.00	33.08
ATOM	2054	CA	LEU	A	260	-0 770	70.900	18.092	1.00	31.90
ATOM	2055	CB	LEU	A	260	-1 543	72.402	16.880	1.00	30 79
ATOM	2056	CG	LEU	A	260	-2 224	72 751	16 957	1 00	33.95
ATOM	2057	CD1	LEU	A	260	-1 342	73 763	17 664	1.00	35 15
ATOM	**2058**	**CD2**	**LEU**	**A**	**260**	**-2.549**	**73.184**	**15.536**	**1.00**	**39.19**
ATOM	2059	C	LEU	A	260	-1.326	69.536	18.470	1 00	33 38
ATOM	2060	O	LEU	A	260	-2 082	69 411	19.420	1 00	35.86
ATOM	2061	N	THR	A	261	-0 988	68 526	17.684	1 00	32 53
ATOM	2062	CA	THR	A	261	-1.480	67 184	17.905	1.00	33 81
ATOM	2063	CB	THR	A	261	-1.571	66.443	16 580	1 00	35.83
ATOM	2064	OG1	THR	A	261	-0 270	66 392	15.977	1 00	33.48
ATOM	2065	CG2	THR	A	261	-2 527	67 155	15.647	1.00	37 64
ATOM	2066	C	THR	A	261	-0 590	66 389	18 840	1.00	39.46
ATOM	2067	O	THR	A	261	-0.651	65.153	18 870	1.00	38.94
ATOM	2068	N	ASN	A	262	0.267	67 094	19.572	1.00	44 29
ATOM	2069	CA	ASN	A	262	1 191	66 456	20.506	1.00	49 58
ATOM	2070	CB	ASN	A	262	0 445	65 952	21.756	1 00	59 13
ATOM	2071	CG	ASN	A	262	1 353	65.841	22.981	1.00	66 86
ATOM	2072	OD1	ASN	A	262	1 367	66 737	23 833	1.00	72 04
ATOM	2073	ND2	ASN	A	262	2.105	64 743	23.081	1.00	67.84
ATOM	2074	C	ASN	A	262	1 941	65 307	19 811	1 00	46 90
ATOM	2075	O	ASN	A	262	2 228	64 274	20.415	1.00	49 43
ATOM	2076	N	ASN	A	263	2.208	65 492	18.522	1 00	41 44
ATOM	2077	CA	ASN	A	263	2 929	64.534	17.698	1 00	37.52
ATOM	2078	C13	ASN	A	263	4 237	64 119	18 347	1 00	41 11
ATOM	2079	CG	ASN	A	263	5 415	64 740	17.670	1 00	47 69
ATOM	2080	OD1	ASN	A	263	5 928	65.764	18 109	1 00	48 68
ATOM	2081	ND2	ASN	A	263	5 824	64.155	16 550	1.00	54 33
ATOM	2082	C	ASN	A	263	2 201	63 322	17 172	1 00	35 18
ATOM	2083	O	ASN	A	263	2 832	62 388	16.679	1 00	34 27
ATOM	2084	N	TYR	A	264	0 877	63 344	17.250	1.00	36 95
ATOM	2085	CA	TYR	A	264	0.063	62.252	16 723	1.00	37.39
TOM	2086	CB	TYR	A	264	-1.393	62.413	17.189	1 00	33.82
ATOM	2087	CG	TYR	A	264	-2 344	61.342	16.713	1 00	33 63
ATOM	2088	CD1	TYR	A	264	-2 446	60 113	17.362	1.00	32 49
ATOM	2089	CE1	TYR	A	264	-3.375	59.151	16.935	1.00	33 06
ATOM	2090	CD2	TYR	A	264	-3.180	61.579	15 627	1.00	37.61
ATOM	2091	CE2	TYR	A	264	-4 105	60.636	15 195	1 00	37.45
ATOM	2092	CZ	TYR	A	264	-4 204	59 429	15 845	1.00	35.62
ATOM	2093	OH	TYR	A	264	-5 169	58 546	15.403	1.00	38.87
ATOM	2094	C	TYR	A	264	0 218	62 311	15.186	1.00	37.01
ATOM	2095	O	TYR	A	264	0.169	61 287	14.499	1.00	37 37
ATOM	2096	N	TYR	A	265	0.390	63.528	14 666	1.00	36 23
ATOM	2097	CA	TYR	A	265	0 642	63.768	13.244	1 00	33 20
ATOM	2098	CB	TYR	A	265	-0 351	64.750	12.640	1 00	26 57
ATOM	2099	CG	TYR	A	265	-1 642	64 115	12.239	1 00	31.72
ATOM	2100	CD1	TYR	A	265	-2 630	64.861	11 610	1.00	33.04
ATOM	2101	CE1	TYR	A	265	-3 854	64.298	11 286	1.00	30 94
ATOM	2102	CD2	TYR	A	265	-1 909	62.775	12 527	1 00	32 98
ATOM	2103	CE2	TYR	A	265	-3 141	62.201	12.207	1 00	31.76
ATOM	2104	CZ	TYR	A	265	-4 102	62 976	11.591	1 00	30.37
ATOM	2105	OH	TYR	A	265	-5 333	62 452	11 312	1 00	38 15
ATOM	2106	C	TYR	A	265	2 028	64.390	13 227	1 00	34 58
ATOM	2107	O	TYR	A	265	2 187	65.586	13 466	1.00	35 29
ATOM	2108	N	LYS	A	266	3 036	63.553	13 022	1.00	34.31
ATOM	2109	CA	LYS	A	266	4 422	63.990	13.002	1.00	33.62
ATOM	2110	CB	LYS	A	266	5.323	62.772	13.039	1.00	39 20
ATOM	2111	CG	LYS	A	266	6 739	63.066	13.491	1.00	56 22
ATOM	2112	CD	LYS	A	266	7 549	61.773	13.584	1.00	67.11
ATOM	2113	CE	LYS	A	266	6.797	60.697	14.372	1.00	74.71

ATOM	2114	NZ	LYS A	266	6.402	61.147	15 748	1.00	80.37
ATOM	2115	C	LYS A	266	4.748	64.784	11 759	1.00	29 29
ATOM	2116	O	LYS A	266	4.184	64.540	10.702	1.00	30 14
ATOM	2117	N	ALA A	267	5.641	65.752	11 890	1.00	26 90
ATOM	2118	CA	ALA A	267	6 063	66.526	10 735	1 00	27.00
ATOM	2119	CB	ALA A	267	6.724	67 809	11 173	1 00	22 67
ATOM	2120	C	ALA A	267	7.079	65.599	10.072	1 00	28 13
ATOM	2121	O	ALA A	267	8 074	65.243	10.695	1.00	31.38
ATOM	2122	N	PRO A	268	6 822	65.155	8 823	1 00	30.02
ATOM	2123	CD	PRO A	268	5 648	65 466	7 989	1 00	29.53
ATOM	2124	Q	PRO A	268	7 732	64 251	8 103	1.00	28.12
ATOM	2125	CB	PRO A	268	7 043	64 081	6 742	1 00	25.57
ATOM	2126	CG	PRO A	268	5 615	64 286	7 035	1.00	25.50
ATOM	2127	C	PRO A	268	9.133	64 805	7 904	1.00	27.55
ATOM	2128	O	PRO A	268	9.281	65.974	7.555	1.00	31.71
ATOM	2129	N	ILE A	269	10 153	63 984	8.156	1 00	26.79
ATOM	2130	Q	ILE A	269	11 549	64.374	7.939	1.00	21.70
ATOM	2131	CB	ILE A	269	12.527	63 535	8 799	1.00	23.68
ATOM	2132	CG2	ILE A	269	13.971	63.768	8 358	1.00	16.90
ATOM	2133	CG1	ILE A	269	12 371	63 881	10.286	1.00	25.36
ATOM	2134	CD1	ILE A	269	12.761	65 311	10.645	1.00	21.95
ATOM	2135	C	ILE A	269	11.788	64.052	6.470	1.00	21.77
ATOM	2136	O	ILE A	269	11.544	62 932	6.025	1.00	23.31
ATOM	2137	N	HIS A	270	12 196	65 043	5.696	1.00	22.73
ATOM	2138	CA	HIS A	270	12 420	64 808	4.280	1.00	21 55
ATOM	2139	CB	HIS A	270	11.161	65.146	3.480	1.00	20 47
ATOM	2140	CG	HIS A	270	10 613	66.507	3.758	1.00	16.63
ATOM	2141	CD2	HIS A	270	10.417	67.570	2.946	1.00	20.91
ATOM	2142	ND1	HIS A	270	10 148	66.885	4.997	1.00	18.74
ATOM	2143	CE1	HIS A	270	9 680	68 .117	4.936	1.00	20 88
ATOM	2144	NE2	HIS A	270	9 828	68.559	3.700	1.00	17.58
ATOM	2145	C	HIS A	270	13 608	65 600	3.783	1.00	22.67
ATOM	2146	O	HIS A	270	14.008	66.588	4.410	1.00	23 83
ATOM	2147	N	ARG A	271	14 201	65.136	2.689	1.00	20 85
ATOM	2148	CA	ARG A	271	15.359	65.797	2.093	1.00	23.79
ATOM	2149	CB	ARG A	271	16 631	65.043	2.461	1.00	22.83
ATOM	2150	CG	ARG A	271	16 615	63.592	2.057	1.00	23.45
ATOM	2151	CD	ARG A	271	17.872	62.894	2.523	1.00	25.22
ATOM	2152	NE	ARG A	271	18 020	61.603	1.862	1.00	26.89
ATOM	2153	CZ	ARG A	271	19.008	60.753	2.103	1.00	25.53
ATOM	2154	NH1	ARG A	271	19 931	61.058	2.996	1.00	29 48
ATOM	2155	NH2	ARG A	271	19 081	59.607	1.441	1.00	25 73
ATOM	2156	C	ARG A	271	15.190	65.873	0.580	1.00	23.68
ATOM	2157	O	ARG A	271	14 319	65.211	0.010	1.00	26.81
ATOM	2158	N	VAL A	272	15 994	66.702	-0.071	1.00	22.19
ATOM	2159	Q	VAL A	272	15.878	66.857	-1.510	1.00	18.76
ATOM	2160	CB	VAL A	272	15.561	68.310	-1.870	1.00	17.63
ATOM	2161	CG1	VAL A	272	15 326	68.446	-3.355	1.00	18 50
ATOM	2162	CG2	VAL A	272	14 340	68.778	-1.107	1.00	15.11
ATOM	2163	C	VAL A	272	17.132	66.418	-2.248	1.00	25.28
ATOM	2164	O	VAL A	272	18.202	66.993	-2.050	1.00	29.40
ATOM	2165	N	LYS A	273	16 985	65.396	-3.092	1.00	27 72
ATOM	2166	CA	LYS A	273	18.059	64.845	-3.919	1.00	25 89
ATOM	2167	CB	LYS A	273	17.572	63.587	-4.645	1.00	27.95
ATOM	2168	CG	LYS A	273	17 355	62 392	-3.753	1.00	31 66
ATOM	2169	CD	LYS A	273	16.404	61 385	-4.376	1.00	35.66
ATOM	2170	CE	LYS A	273	16 963	60.740	-5.621	1.00	41 21
ATOM	2171	NZ	LYS A	273	16 185	59 514	-5.974	1.00	42.41
ATOM	2172	C	LYS A	273	18.551	65 837	-4.968	1.00	25.96
ATOM	2173	O	LYS A	273	17 784	66 653	-5.486	1.00	26 05
ATOM	2174	N	TRP A	274	19 843	65 759	-5.268	1.00	25 99
ATOM	2175	Q	TRP A	274	20.489	66 616	-6.267	1.00	24 01
ATOM	2176	CB	TRP A	274	21 975	66 623	-6.096	1.00	24.20
ATOM	2177	CG	TRP A	274	22.700	67 347	-7.187	1.00	23.66
ATOM	2178	CD2	TRP A	274	23.526	66 762	-8.194	1.00	21.71
ATOM	2179	CE2	TRP A	274	23.997	67 812	-9.008	1.00	21.28
ATOM	2180	CE3	TRP A	274	23.900	65.453	-8.498	1.00	25.08
ATOM	2181	CD1	TRP A	274	22.709	68.689	-7.417	1.00	26.21
ATOM	2182	NE1	TRP A	274	23.490	68.979	-8.509	1.00	28.27
ATOM	2183	CZ2	TRP A	274	24.839	67.594	-10.089	1.00	23.56
ATOM	2184	CZ3	TRP A	274	24.739	65.237	-9.582	1.00	29.23
ATOM	2185	CH2	TRP A	274	25.193	66.305	-10.367	1.00	24.09
ATOM	2186	C	TRP A	274	20.105	66.099	-7.653	1.00	27.26

ATOM	2187	C	TRP	A	274	20.357	64.938	-7.970	1.00	32.63
ATOM	2188	N	VAL	A	275	19.503	66.964	-8.461	1.00	28.27
ATOM	2189	CA	VAL	A	275	19.110	66.636	-9.825	1.00	25.56
ATOM	2190	CB	VAL	A	275	17.582	66 606	-9.971	1 00	23.27
ATOM	2191	CG1	VAL	A	275	17.200	66 358	-11.410	1 00	23.05
ATOM	2192	CG2	VAL	A	275	16.993	65 545	-9.073	1 00	25.58
ATOM	2193	C	VAL	A	275	19.645	67 760	-10.689	1 00	23.04
ATOM	2194	O	VAL	A	275	19.194	68.884	-10 573	1 00	27.65
ATOM	2195	N	ASN	A	276	20.627	67.480	-11 532	1 00	24.79
ATOM	2196	CA	ASN	A	276	21.172	68 539	-12 372	1 00	23.43
ATOM	2197	CB	ASN	A	276	22.626	68 262	-12 737	1 00	23.64
ATOM	2198	CG	ASN	A	276	23.237	69.374	-13 563	1 00	27.31
ATOM	2199	OD1	ASN	A	276	22.697	70.479	-13 650	1 00	25.48
ATOM	2200	ND2	ASN	A	276	24.382	69 096	-14 156	1 00	32.14
ATOM	2201	C	ASN	A	276	20.347	68.732	-13.632	1 00	24.63
ATOM	2202	O	ASN	A	276	20.683	68.215	-14 694	1 00	31 02
ATOM	2203	N	ALA	A	277	19 244	69 453	-13.499	1.00	25 78
ATOM	**2204**	**CA**	**ALA**	**A**	**277**	**18.364**	**69.719**	**-14.620**	**1.00**	**23.03**
ATOM	2205	CB	ALA	A	277	17 502	68.507	-14.911	1 00	26.09
ATOM	2206	C	ALA	A	277	17 490	70 903	-14.288	1.00	25 78
ATOM	2207	O	ALA	A	277	17 232	71.177	-13.119	1.00	27 01
ATOM	2208	N	GLU	A	278	17 034	71 602	-15.321	1.00	25 92
ATOM	2209	CA	GLU	A	278	16 176	72.760	-15.139	1 00	27 97
ATOM	2210	CB	GLU	A	278	16 111	73 616	-16 399	1 00	29 38
ATOM	2211	CG	GLU	A	278	17.326	74 473	-16 634	1 00	34.40
ATOM	2212	CD	GLU	A	278	17 373	75.697	-15 764	1 00	31.39
ATOM	2213	OE1	GLU	A	278	16 312	76 182	-15 327	1.00	35.93
ATOM	2214	OE2	GLU	A	278	18 489	76 186	-15.537	1 00	37 93
ATOM	2215	C	GLU	A	278	14 777	72 323	-14 767	1 00	30 01
ATOM	2216	O	GLU	A	278	13 999	71 867	-15 601	1 00	33 28
ATOM	2217	N	ARG	A	279	14 485	72 419	-13 487	1 00	30 78
ATOM	2218	CA	ARG	A	279	13 185	72 069	-12.986	1 00	29.39
ATOM	2219	CB	ARG	A	279	13.232	70 718	-12.294	1.00	29 88
ATOM	2220	CG	ARG	A	279	13 756	69.606	-13.168	1.00	29.15
ATOM	2221	CD	ARG	A	279	12 891	69.382	-14 381	1.00	26.70
ATOM	2222	NE	ARG	A	279	13 340	68.183	-15 073	1 00	28.42
ATOM	2223	CZ	ARG	A	279	13 978	68 185	-16.234	1 00	25.05
ATOM	2224	NH1	ARG	A	279	14 224	69 324	-16.855	1.00	21.11
ATOM	2225	NH2	ARG	A	279	14 477	67 059	-16.716	1 00	26.84
ATOM	2226	C	ARG	A	279	12 813	73 163	-12.007	1 00	30.45
ATOM	2227	O	ARG	A	279	13 645	74 001	-11 643	1 00	28.64
ATOM	2228	N	GLN	A	280	11 560	73.147	-11 583	1.00	31.12
ATOM	2229	CA	GLN	A	280	11 045	74 134	-10 661	1.00	33.15
ATOM	2230	CB	GLN	A	280	10.260	75.182	-11.427	1.00	38.18
ATOM	2231	CG	GLN	A	280	9 171	74.580	-12.286	1.00	53.46
ATOM	2232	CD	GLN	A	280	8 596	75.565	-13 278	1.00	57.41
ATOM	2233	OE1	GLN	A	280	9 209	76.593	-13.568	1.00	60.52
ATOM	2234	NE2	GLN	A	280	7.418	75.250	-13.820	1.00	60.10
ATOM	2235	C	GLN	A	280	10.139	73 430	-9 679	1.00	30.33
ATOM	2236	O	GLN	A	280	9.602	72.363	-9.975	1.00	32.02
ATOM	2237	N	SER	A	281	9.958	74.049	-8 521	1.00	26.28
ATOM	2238	CA	SER	A	281	9.131	73.510	-7 462	1.00	18.83
ATOM	2239	CB	SER	A	281	10.034	72.908	-6.390	1.00	16.21
ATOM	2240	OG	SER	A	281	9.281	72.175	-5 458	1 00	31.28
ATOM	2241	C	SER	A	281	8.344	74.691	-6.918	1 00	17.91
ATOM	2242	O	SER	A	281	8.870	75.796	-6 852	1 00	15.21
ATOM	2243	N	LEU	A	282	7.070	74.487	-6 596	1 00	24.14
ATOM	2244	CA	LEU	A	282	6.239	75.578	-6.068	1.00	24.06
ATOM	2245	CB	LEU	A	282	5.224	76.049	-7.098	1 00	26.03
ATOM	2246	CG	LEU	A	282	5.733	76.662	-8.388	1 00	34.69
ATOM	2247	CD1	LEU	A	282	6.212	75.564	-9.339	1.00	37 28
ATOM	2248	CD2	LEU	A	282	4.582	77.421	-9.009	1.00	38 00
ATOM	2249	C	LEU	A	282	5.480	75.182	-4.814	1.00	23 88
ATOM	2250	O	LEU	A	282	4.368	74.652	-4.894	1.00	21 16
ATOM	2251	N	PRO	A	283	6.109	75.372	-3.637	1 00	22 81
ATOM	2252	CD	PRO	A	283	7.531	75.682	-3.434	1 00	22 38
ATOM	2253	CA	PRO	A	283	5.463	75.035	-2.372	1 00	20 82
ATOM	2254	CB	PRO	A	283	6.661	74.739	-1.472	1 00	18.71
ATOM	2255	CG	PRO	A	283	7.663	75.746	-1.928	1 00	19 17
ATOM	2256	C	PRO	A	283	4.651	76.192	-1.847	1 00	17 56
ATOM	2257	O	PRO	A	283	5.023	77.349	-2.001	1 00	19 99
ATOM	2258	N	PHE	A	284	3.496	75.874	-1.282	1.00	18 04
ATOM	2259	CA	PHE	A	284	2.628	76.869	-0.686	1.00	14.83

ATOM	2260	CB	PHE A	284	1.202	76.739	-1.221	1.00	13.11
ATOM	2261	CG	PHE A	284	0.222	77.695	-0.590	1.00	9.51
ATOM	2262	CD1	PHE A	284	0.361	79.072	-0.757	1 00	7.91
ATOM	2263	CD2	PHE A	284	-0.840	77.218	0.176	1.00	8.25
ATOM	2264	CE1	PHE A	284	-0.546	79.963	-0.172	1 00	9.04
ATOM	2265	CE2	PHE A	284	-1.755	78.103	0.769	1.00	7.90
ATOM	2266	CZ	PHE A	284	-1.607	79 480	0.596	1 00	7.48
ATOM	2267	C	PHE A	284	2.657	76 481	0.777	1.00	15.38
ATOM	2268	O	PHE A	284	2.315	75.351	1.126	1 00	13 28
ATOM	2269	N	PHE A	285	3.130	77.381	1.625	1.00	11 26
ATOM	2270	CA	PHE A	285	3.204	77.096	3.045	1 00	11.08
ATOM	2271	CB	PHE A	285	4 488	77.682	3.622	1 00	11 89
ATOM	2272	CG	PHE A	285	5 734	77.103	3.021	1 00	13.37
ATOM	2273	CD1	PHE A	285	6 418	77 779	2.024	1.00	12 80
ATOM	2274	CD2	PHE A	285	6 229	75 882	3.458	1.00	14.08
ATOM	2275	CE1	PHE A	285	7.584	77 245	1.477	1.00	16 30
ATOM	2276	CE2	PHE A	285	7.396	75 347	2.911	1 00	13.47
ATOM	2277	CZ	PHE A	285	8 066	76.030	1.925	1 00	7 59
ATOM	2278	C	PHE A	285	1 985	77.644	3.756	1.00	12 95
ATOM	2279	O	PHE A	285	1.781	78.863	3.801	1.00	14.08
ATOM	2280	N	VAL A	286	1.150	76 746	4.271	1.00	11.34
ATOM	2281	CA	VAL A	286	-0 062	77.158	4.969	1 00	15.20
ATOM	2282	CB	VAL A	286	-1.128	76.021	4.997	1 00	13 61
ATOM	2283	CG1	VAL A	286	-2.365	76.467	5.739	1 00	11.57
ATOM	2284	CG2	VAL A	286	-1 511	75.629	3.587	1 00	10.57
ATOM	2285	C	VAL A	286	0 271	77.647	6.384	1.00	18.76
ATOM	2286	O	VAL A	286	0.667	76.876	7.257	1 00	24.10
ATOM	2287	N	ASN A	287	0.190	78.955	6.571	1.00	17 87
ATOM	2288	CA	ASN A	287	0.461	79.568	7.850	1 00	18 13
ATOM	2289	CB	ASN A	287	1 570	80.621	7.722	1.00	19.63
ATOM	2290	CG	ASN A	287	2.940	80.017	7.427	1.00	17.67
ATOM	2291	OD1	ASN A	287	3.287	78.940	7.907	1.00	15.97
ATOM	2292	ND2	ASN A	287	3 729	80.727	6.644	1 00	19 12
ATOM	2293	C	ASN A	287	-0 844	80.242	8.229	1 00	21 86
ATOM	2294	O	ASN A	287	-1.584	80.680	7 347	1.00	26.85
ATOM	2295	N	LEU A	288	-1 148	80.302	9.523	1 00	19.51
ATOM	2296	CA	LEU A	288	-2 374	80.928	9.979	1 00	14 83
ATOM	2297	CB	LEU A	288	-2.853	80.254	11.253	1 00	12.62
ATOM	2298	CG	LEU A	288	-2.982	78.741	11.075	1.00	17.68
ATOM	2299	CD1	LEU A	288	-3.540	78.114	12 332	1.00	16.20
ATOM	2300	CD2	LEU A	288	-3.883	78.428	9 909	1 00	14 63
ATOM	2301	C	LEU A	288	-2 139	82.414	10 188	1 00	16.91
ATOM	2302	O	LEU A	288	-1.218	82.981	9.611	1.00	20.51
ATOM	2303	N	GLY A	289	-2.974	83.051	10.996	1.00	16.67
ATOM	2304	CA	GLY A	289	-2.823	84.473	11.240	1.00	15.37
ATOM	2305	C	GLY A	289	-1.831	84 700	12.350	1.00	19.82
ATOM	2306	O	GLY A	289	-1.571	83 795	13.130	1.00	22.79
ATOM	2307	N	TYR A	290	-1.342	85.924	12 477	1.00	19.69
ATOM	2308	CA	TYR A	290	-0.354	86.246	13.491	1.00	23.55
ATOM	2309	CB	TYR A	290	0.058	87 705	13.359	1.00	22.89
ATOM	2310	CG	TYR A	290	1.265	88 073	14 184	1.00	30.95
ATOM	2311	CD1	TYR A	290	2.558	87.793	13 730	1.00	31.65
ATOM	2312	CE1	TYR A	290	3.671	88.142	14 481	1.00	32.74
ATOM	2313	CD2	TYR A	290	1.122	88.710	15 414	1.00	29.60
ATOM	2314	CE2	TYR A	290	2.228	89.063	16.172	1.00	31.69
ATOM	2315	CZ	TYR A	290	3.494	88.778	15 699	1.00	32.60
ATOM	2316	OH	TYR A	290	4.587	89.149	16 435	1.00	38.35
ATOM	2317	C	TYR A	290	-0.825	85.973	14 912	1.00	26.88
ATOM	2318	O	TYR A	290	-0.064	85.469	15 747	1.00	32.22
ATOM	2319	N	ASP A	291	-2.080	86.302	15 180	1.00	32.16
ATOM	2320	CA	ASP A	291	-2.650	86.121	16 505	1.00	34.89
ATOM	2321	CB	ASP A	291	-3 621	87.271	16.809	1.00	44.67
ATOM	2322	CG	ASP A	291	-2 907	88.607	17.064	1 00	54 47
ATOM	2323	OD1	ASP A	291	-1 678	88.612	17.294	1 00	62.50
ATOM	2324	OD2	ASP A	291	-3 583	89.662	17.057	1 00	59.68
ATOM	2325	C	ASP A	291	-3 341	84.786	16.743	1 00	33.13
ATOM	2326	O	ASP A	291	-3 867	84.552	17.828	1 00	36.71
ATOM	2327	N	SER A	292	-3 325	83.902	15.755	1.00	32.93
ATOM	2328	CA	SER A	292	-3.989	82.611	15.896	1.00	33.04
ATOM	2329	CB	SER A	292	-4.074	81.892	14.551	1.00	32.62
ATOM	2330	OG	SER A	292	-4.870	82.629	13.641	1.00	37.64
ATOM	2331	C	SER A	292	-3.394	81.675	16.933	1.00	33.50
ATOM	2332	O	SER A	292	-2.223	81.310	16.870	1.00	35.88

ATOM	2333	N	VAL A	293	-4.223	81.283	17.889	1.00	35.69
ATOM	2334	CA	VAL A	293	-3.807	80.371	18.936	1.00	33.43
ATOM	2335	CB	VAL A	293	-3.867	81.015	20.333	1.00	28.87
ATOM	2336	CG1	VAL A	293	-3.244	80.086	21.346	1.00	29.10
ATOM	2337	CG2	VAL A	293	-3.157	82.350	20.340	1.00	28.79
ATOM	2338	C	VAL A	293	-4.754	79.193	18.925	1.00	33.08
ATOM	2339	O	VAL A	293	-5.971	79.366	18.990	1.00	33.77
ATOM	2340	N	ILE A	294	-4.187	78.002	18.790	1.00	34.36
ATOM	2341	CA	ILE A	294	-4.952	76.770	18.784	1.00	33.14
ATOM	2342	CB	ILE A	294	-4.754	76.000	17.458	1.00	33.14
ATOM	2343	CG2	ILE A	294	-5.426	74.629	17.518	1.00	28.09
ATOM	2344	CG1	ILE A	294	-5.318	76.832	16.303	1.00	29.00
ATOM	2345	CD1	ILE A	294	-5.328	76.129	14.973	1.00	30.92
ATOM	2346	C	ILE A	294	-4.476	75.952	19.983	1.00	36.82
ATOM	2347	O	ILE A	294	-3.277	75.882	20.273	1.00	40.13
ATOM	2348	N	ASP A	295	-5.427	75.385	20.710	1.00	37.77
ATOM	2349	CA	ASP A	295	-5.124	74.604	21.889	1.00	36.56
ATOM	**2350**	**CB**	**ASP A**	**295**	**-6.346**	**74.499**	**22.783**	**1.00**	**42.24**
ATOM	2351	CG	ASP A	295	-6.163	75.234	24.071	1.00	50.87
ATOM	2352	OD1	ASP A	295	-6.049	74.565	25.117	1.00	60.02
ATOM	2353	OD2	ASP A	295	-6.092	76.481	24.038	1.00	55.86
ATOM	2354	C	ASP A	295	-4.655	73.223	21.544	1.00	35.69
ATOM	2355	O	ASP A	295	-5.384	72.453	20.928	1.00	35.08
ATOM	2356	N	PRO A	296	-3.431	72.879	21.955	1.00	35.13
ATOM	2357	CD	PRO A	296	-2.488	73.736	22.692	1.00	34.11
ATOM	2358	CA	PRO A	296	-2.847	71.563	21.690	1.00	35.32
ATOM	2359	CB	PRO A	296	-1.478	71.653	22.368	1.00	33.77
ATOM	2360	CG	PRO A	296	-1.169	73.116	22.339	1.00	35.72
ATOM	2361	C	PRO A	296	-3.689	70.463	22.327	1.00	38.35
ATOM	2362	O	PRO A	296	-4.269	70.653	23.394	1.00	42.07
ATOM	2363	N	PHE A	297	-3.706	69.300	21.697	1.00	38.55
ATOM	2364	CA	PHE A	297	-4.455	68.180	22.208	1.00	37.27
ATOM	2365	CB	PHE A	297	-5.877	68.209	21.654	1.00	34.45
ATOM	2366	CG	PHE A	297	-5.957	68.187	20.151	1.00	31.82
ATOM	2367	CD1	PHE A	297	-6.324	67.025	19.475	1.00	30.97
ATOM	2368	CD2	PHE A	297	-5.712	69.339	19.414	1.00	31.48
ATOM	2369	CE1	PHE A	297	-6.445	67.018	18.083	1.00	30.11
ATOM	2370	CE2	PHE A	297	-5.832	69.338	18.023	1.00	29.97
ATOM	2371	CZ	PHE A	297	-6.200	68.177	17.358	1.00	30.13
ATOM	2372	C	PHE A	297	-3.770	66.887	21.809	1.00	40.88
ATOM	2373	O	PHE A	297	-2.954	66.865	20.891	1.00	43.86
ATOM	2374	N	ASP A	298	-4.064	65.806	22.511	1.00	44.53
ATOM	2375	CA	ASP A	298	-3.466	64.534	22.167	1.00	48.48
ATOM	2376	CB	ASP A	298	-2.590	64.015	23.295	1.00	52.93
ATOM	2377	CG	ASP A	298	-1.808	62.778	22.898	1.00	57.44
ATOM	2378	OD1	ASP A	298	-2.020	62.254	21.778	1.00	54.35
ATOM	2379	OD2	ASP A	298	-0.964	62.333	23.705	1.00	66.50
ATOM	2380	C	ASP A	298	-4.584	63.552	21.907	1.00	50.22
ATOM	2381	O	ASP A	298	-5.215	63.067	22.827	1.00	49.77
ATOM	2382	N	PRO A	299	-4.789	63.199	20.630	1.00	52.46
ATOM	2383	CD	PRO A	299	-4.105	63.730	19.439	1.00	52.72
ATOM	2384	CA	PRO A	299	-5.835	62.266	20.230	1.00	56.64
ATOM	2385	CB	PRO A	299	-5.663	62.206	18.717	1.00	54.35
ATOM	2386	CG	PRO A	299	-5.165	63.564	18.388	1.00	50.07
ATOM	2387	C	PRO A	299	-5.648	60.898	20.868	1.00	63.86
ATOM	2388	O	PRO A	299	-6.492	60.011	20.687	1.00	69.53
ATOM	2389	N	MG A	300	-4.535	60.712	21.580	1.00	68.69
ATOM	2390	CA	ARG A	300	-4.231	59.449	22.250	1.00	73.13
ATOM	2391	CB	ARG A	300	-2.731	59.153	22.191	1.00	73.05
ATOM	2392	CG	ARG A	300	-2.202	58.825	20.810	1.00	75.18
ATOM	2393	CD	ARG A	300	-0.682	58.842	20.790	1.00	72.55
ATOM	2394	NE	ARG A	300	-0.165	60.144	21.181	1.00	71.35
ATOM	2395	CZ	ARG A	300	0.867	60.748	20.595	1.00	71.94
ATOM	2396	NH1	ARG A	300	1.506	60.171	19.579	1.00	73.46
ATOM	2397	NH2	ARG A	300	1.274	61.934	21.032	1.00	71.10
ATOM	2398	C	ARG A	300	-4.685	59.414	23.708	1.00	76.43
ATOM	2399	O	ARG A	300	-4.552	58.390	24.374	1.00	80.12
ATOM	2400	N	GLU A	301	-5.202	60.536	24.196	1.00	77.10
ATOM	2401	CA	GLU A	301	-5.687	60.596	25.562	1.00	81.37
ATOM	2402	CB	GLU A	301	-4.984	61.711	26.331	1.00	82.38
ATOM	2403	CG	GLU A	301	-3.474	61.523	26.422	1.00	89.06
ATOM	2404	CD	GLU A	301	-2.918	62.004	27.750	1.00	94.30
ATOM	2405	OE1	GLU A	301	-3.152	63.179	28.125	1.00	97.83

ATOM	2406	OE2	GLU A	301	-2 241	61 201	28.425	1.00	97.36
ATOM	2407	C	GLU A	301	-7.193	60 781	25 642	1.00	84.64
ATOM	2408	O	GLU A	301	-7 779	61 498	24 836	1.00	83.56
ATOM	2409	N	PRO A	302	-7.949	60.122	26.611	1.00	88.29
ATOM	2410	CD	PRO A	302	-7.263	59 114	27 527	1.00	89.03
ATOM	2411	CA	PRO A	302	-9 303	60 201	26.800	1.00	87.98
ATOM	2412	CB	PRO A	302	-9 521	59.416	28.095	1.00	88.81
ATOM	2413	CG	PRO A	302	-8 478	58 337	27 978	1 00	88.81
ATOM	2414	C	PRO A	302	-9.804	61 652	26 925	1 00	86.15
ATOM	2415	O	PRO A	302	-10 737	62.060	26.236	1 00	85 57
ATOM	2416	N	ASN A	303	-9 184	62.425	27 817	1.00	84.86
ATOM	2417	CA	ASN A	303	-9.563	63 822	27.985	1 00	85.24
ATOM	2418	CB	ASN A	303	-8.929	64 404	29.254	1.00	89.02
ATOM	2419	CG	ASN A	303	-9.217	65.900	29.433	1 00	93.08
ATOM	2420	OD1	ASN A	303	-8 501	66.589	30.150	1.00	95 61
ATOM	2421	ND2	ASN A	303	-10 242	66.401	28.755	1.00	95 94
ATOM	2422	C	ASN A	303	-9 073	64.602	26.773	1.00	83.46
ATOM	2423	O	ASN A	303	-9.678	65 601	26.377	1.00	82.51
ATOM	2424	N	GLY A	304	-8 001	64.099	26.169	1.00	82.29
ATOM	2425	CA	GLY A	304	-7 413	64 745	25.016	1.00	79 23
ATOM	2426	C	GLY A	304	-6 639	65.945	25.513	1.00	77 89
ATOM	2427	O	GLY A	304	-6 503	66 945	24.802	1.00	78 97
ATOM	2428	N	LYS A	305	-6.156	65.855	26.748	1.00	76.87
ATOM	2429	CA	LYS A	305	-5.403	66.938	27.348	1.00	76 76
ATOM	2430	CB	LYS A	305	-5 585	66.962	28.880	1.00	78 46
ATOM	2431	CG	LYS A	305	-4.408	66.440	29.691	1.00	82.23
ATOM	2432	CD	LYS A	305	-3.751	67.539	30.519	1.00	85 07
ATOM	2433	CE	LYS A	305	-2.573	66.997	31.311	1.00	88.93
ATOM	2434	NZ	LYS A	305	-2 157	67.917	32.403	1 00	93 14
ATOM	2435	C	LYS A	305	-3.949	66.755	26.972	1.00	73.92
ATOM	2436	O	LYS A	305	-3.474	65.623	26.867	1.00	73.27
ATOM	2437	N	SER A	306	-3.237	67.855	26.797	1.00	72.39
ATOM	2438	CA	SER A	306	-1 844	67.787	26.417	1 00	73.15
ATOM	2439	CB	SER A	306	-1 656	68.461	25.061	1 00	72.57
ATOM	2440	OG	SER A	306	-2.237	69.762	25.069	1.00	70 16
ATOM	2441	C	SER A	306	-0.982	68.474	27.445	1.00	73.60
ATOM	2442	O	SER A	306	-1 481	69.180	28.328	1.00	71.26
ATOM	2443	N	ASP A	307	0 314	68.208	27.363	1.00	76.59
ATOM	2444	CA	ASP A	307	1.281	68.827	28.260	1.00	78 33
ATOM	2445	CB	ASP A	307	2.480	67.891	28.515	1 00	84.92
ATOM	2446	CG	ASP A	307	3 022	67.239	27.236	1.00	89.57
ATOM	2447	OD1	ASP A	307	3 809	67.902	26.515	1 00	90 72
ATOM	2448	OD2	ASP A	307	2.672	66.065	26.956	1 00	90.72
ATOM	2449	C	ASP A	307	1 734	70.130	27.593	1.00	74.93
ATOM	2450	O	ASP A	307	1 883	71.163	28.254	1.00	73.18
ATOM	2451	N	ARG A	308	1 893	70.072	26.268	1.00	70.05
ATOM	2452	CA	ARG A	308	2 327	71.212	25.471	1.00	64.62
ATOM	2453	CB	ARG A	308	2.295	70.877	23.986	1.00	64.91
ATOM	2454	CG	ARG A	308	3.177	69.738	23.570	1.00	65.23
ATOM	2455	CD	ARG A	308	3 284	69.720	22.067	1.00	65.31
ATOM	2456	NE	ARG A	308	3 889	68.494	21.573	1.00	68.52
ATOM	2457	CZ	ARG A	308	5 145	68.139	21.800	1.00	69.44
ATOM	2458	NH1	ARG A	308	5 939	68.925	22.515	1.00	70.73
ATOM	2459	NH2	ARG A	308	5.596	66.983	21.334	1.00	71.60
ATOM	2460	C	ARG A	308	1 422	72.394	25.695	1.00	60.56
ATOM	2461	O	ARG A	308	0.211	72.243	25.786	1.00	62.91
ATOM	2462	N	GLU A	309	2.016	73.576	25.721	1.00	58.75
ATOM	2463	CA	GLU A	309	1.278	74.807	25.937	1.00	59.53
ATOM	2464	CB	GLU A	309	2 155	75.795	26.707	1 00	64.51
ATOM	2465	CG	GLU A	309	2 863	75.195	27.909	1 00	72.73
ATOM	2466	CD	GLU A	309	4.037	76.041	28.375	1 00	78.39
ATOM	2467	OE1	GLU A	309	5 196	75.650	28.107	1.00	80.45
ATOM	2468	OE2	GLU A	309	3 802	77.091	29.013	1 00	81.42
ATOM	2469	C	GLU A	309	0 895	75.423	24.595	1.00	58 18
ATOM	2470	O	GLU A	309	1.550	75.172	23.576	1.00	56 69
ATOM	2471	N	PRO A	310	-0 202	76.204	24.566	1.00	57 07
ATOM	2472	CD	PRO A	310	-1.130	76.528	25.662	1.00	58 98
ATOM	2473	CA	PRO A	310	-0.639	76.848	23.325	1.00	54 68
ATOM	2474	CB	PRO A	310	-1.898	77.610	23.755	1.00	56.45
ATOM	2475	CG	PRO A	310	-1.671	77.867	25.214	1.00	57.32
ATOM	2476	C	PRO A	310	0.456	77.787	22.831	1.00	49.05
ATOM	2477	O	PRO A	310	1.136	78.437	23.631	1.00	48.09
ATOM	2478	N	LEU A	311	0.617	77.835	21.512	1.00	43.40

ATOM	2479	CA	LEU A	311	1.626	78.650	20.859	1.00	36.12
ATOM	2480	CB	LEU A	311	2.661	77.726	20.204	1.00	32.22
ATOM	2481	CG	LEU A	311	3.919	78.324	19.578	1.00	31.79
ATOM	2482	CD1	LEU A	311	4.582	79.300	20.539	1.00	28.33
ATOM	2483	CD2	LEU A	311	4.862	77.194	19.229	1.00	26.30
ATOM	2484	C	LEU A	311	0.936	79.478	19.793	1.00	32.51
ATOM	2485	O	LEU A	311	0.300	78.915	18.903	1.00	35.00
ATOM	2486	N	SER A	312	1.012	80.804	19.899	1.00	27.12
ATOM	2487	CA	SER A	312	0.386	81.654	18.894	1.00	26.22
ATOM	2488	CB	SER A	312	0.324	83.123	19.339	1 00	22 14
ATOM	2489	OG	SER A	312	1.479	83.859	19.000	1 00	31 44
ATOM	2490	C	SER A	312	1.205	81 464	17.621	1 00	30 09
ATOM	2491	O	SER A	312	2.438	81 349	17.671	1.00	34 62
ATOM	2492	N	TYR A	313	0.526	81 399	16.483	1 00	30.05
ATOM	2493	CA	TYR A	313	1 208	81 164	15 222	1 00	26.78
ATOM	2494	CB	TYR A	313	0.221	81 101	14 070	1 00	21 90
ATOM	2495	CG	TYR A	313	0 740	80 223	12 968	1.00	23 94
ATOM	2496	CD1	TYR A	313	0.464	78 868	12.972	1.00	20.72
ATOM	2497	CE1	TYR A	313	0 991	78 032	12.022	1 00	22.06
ATOM	2498	CD2	TYR A	313	1 555	80 729	11.951	1 00	26 61
ATOM	2499	CE2	TYR A	313	2 091	79 891	10 996	1 00	26.69
ATOM	2500	CZ	TYR A	313	1 792	78 541	11 041	1 00	17.14
ATOM	2501	OH	TYR A	313	2 294	77 666	10.123	1 00	24.17
ATOM	2502	C	TYR A	313	2 299	82 153	14.895	1.00	25 77
ATOM	2503	O	TYR A	313	3.326	81 778	14 334	1 00	23.63
ATOM	2504	N	GLY A	314	2 071	83.415	15.238	1.00	28 58
ATOM	2505	CA	GLY A	314	3 053	84 444	14.965	1.00	34 94
ATOM	2506	C	GLY A	314	4 370	84 186	15.674	1.00	37.23
ATOM	2507	O	GLY A	314	5.434	84.453	15 117	1.00	41.94
ATOM	2508	N	ASP A	315	4 301	83 683	16 906	1 00	37.16
ATOM	2509	CA	ASP A	315	5 498	83 388	17.682	1.00	33 44
ATOM	2510	CB	ASP A	315	5.162	83.140	19.157	1 00	37.41
ATOM	2511	CG	ASP A	315	4 707	84.406	19 881	1.00	40 95
ATOM	2512	OD1	ASP A	315	3.906	84 295	20 835	1 00	48.93
ATOM	2513	OD2	ASP A	315	5.147	85.515	19 504	1.00	45.51
ATOM	2514	C	ASP A	315	6.147	82.172	17.074	1.00	28.81
ATOM	2515	O	ASP A	315	7.357	82.139	16 893	1 00	32 18
ATOM	2516	N	TYR A	316	5 333	81 179	16.746	1.00	26.31
ATOM	2517	CA	TYR A	316	5.823	79 963	16.116	1.00	25 28
ATOM	2518	CB	TYR A	316	4 646	79 064	15 709	1.00	23 80
ATOM	2519	CG	TYR A	316	4 986	77 997	14 682	1 00	28.01
ATOM	2520	CD1	TYR A	316	5 604	76.802	15 061	1.00	26 83
ATOM	2521	CE1	TYR A	316	5.903	75.810	14.106	1.00	25.18
ATOM	2522	CD2	TYR A	316	4.682	78 177	13.323	1 00	22 23
ATOM	2523	CE2	TYR A	316	4 981	77.194	12 372	1 00	16.07
ATOM	2524	CZ	TYR A	316	5 586	76 020	12.769	1 00	19.33
ATOM	2525	08	TYR A	316	5 850	75.040	11 843	1.00	22.12
ATOM	2526	C	TYR A	316	6 625	80 333	14 872	1 00	26.20
ATOM	2527	O	TYR A	316	7 812	80 010	14 766	1 00	23 86
ATOM	2528	N	LEU A	317	5 977	81 062	13 966	1.00	26 87
ATOM	2529	CA	LEU A	317	6 579	81.454	12 705	1 00	26 33
ATOM	2530	CB	LEU A	317	5.548	82.112	11 783	1 00	22.99
ATOM	2531	CG	LEU A	317	6 031	82 167	10 334	1 00	17.66
ATOM	2532	CD1	LEU A	317	5 962	80 780	9.722	1 00	16 43
ATOM	2533	CD2	LEU A	317	5 205	83.147	9 549	1 00	13 47
ATOM	2534	C	LEU A	317	7 801	82 340	12 830	1 00	25 42
ATOM	2535	O	LEU A	317	8 781	82 125	12.134	1.00	29.40
ATOM	2536	N	GLN A	318	7.753	83 341	13 696	1 00	26.38
ATOM	2537	CA	GLN A	318	8 891	84 226	13.846	1.00	29 10
ATOM	2538	CB	GLN A	318	8 643	85 254	14 933	1 00	34.57
ATOM	2539	CG	GLN A	318	7.722	86 361	14.557	1 00	45 89
ATOM	2540	CD	GLN A	318	7 422	87 230	15 744	1 00	54 11
ATOM	2541	OE1	GLN A	318	8 276	87 996	16 198	1 00	60 92
ATOM	2542	NE2	GLN A	318	6.224	87 084	16.292	1 00	56 69
ATOM	2543	C	GLN A	318	10 114	82 429	14.215	1 00	32 19
ATOM	2544	O	GLN A	318	11 147	83 529	13.560	1 00	34 97
ATOM	2545	N	ASN A	319	9 967	82 589	15.231	1 00	33.42
ATOM	2546	CA	ASN A	319	11 076	81.780	15.711	1 00	38 92
ATOM	2547	CB	ASN A	319	10 751	81.192	17.088	1 00	45.44
ATOM	2548	CG	ASN A	319	10 635	82.276	18.174	1 00	54 83
ATOM	2549	OD1	ASN A	319	11 612	82.952	18.502	1 00	56 44
ATOM	2550	ND2	ASN A	319	9 429	82.470	18.702	1.00	59 48
ATOM	2551	C	ASN A	319	11 506	80.705	14.725	1.00	40.03

ATOM	2552	O	ASN A	319	12.703	80.502	14.494	1.00	44 50
ATOM	2553	N	GLY A	320	10.531	80 058	14.100	1.00	39 74
ATOM	2554	CA	GLY A	320	10.827	79 022	13.130	1 00	35 73
ATOM	2555	C	GLY A	320	11. 611	79 582	11 .962	1 00	35 37
ATOM	2556	O	GLY A	320	12.536	78 952	11.471	1 00	37.50
ATOM	2557	N	LEU A	321	11 270	80 786	11. 530	1 00	34 76
ATOM	2558	CA	LEU A	321	11.967	81 393	10 415	1.00	39 63
ATOM	2559	CB	LEU A	321	12.191	82 583	9 877	1.00	36.97
ATOM	2560	CG	LEU A	321	9 901	82.168	9 187	1.00	38 18
ATOM	2561	CD1	LEU A	321	9.271	83.392	8.570	1 00	38.33
ATOM	2562	CD2	LEU A	321	10.181	81.108	8 134	1 00	35.19
ATOM	2563	C	LEU A	321	13.382	81 805	10 757	1 00	44.08
ATOM	2564	O	LEU A	321	14.287	81 606	9 953	1.00	46 65
ATOM	2565	N	VAL A	322	13.581	82 378	11.941	1.00	49 49
ATOM	2566	CA	VAL A	322	14.923	82 806	12.345	1.00	53 83
ATOM	2567	CB	VAL A	322	14.939	83 617	13.671	1 00	53.89
ATOM	2568	CG1	VAL A	322	13.945	84 767	13 615	1 00	53 18
ATOM	2569	CG2	VAL A	322	14.698	82.698	14 869	1.00	55.17
ATOM	2570	C	VAL A	322	15.894	81 645	12.511	1.00	54.31
ATOM	2571	O	VAL A	322	17.104	81.848	12 478	1.00	59.46
ATOM	2572	N	SER A	323	15.378	80.452	12.773	1.00	52 61
ATOM	2573	CA	SER A	323	16.254	79.309	12.940	1.00	53 68
ATOM	2574	CB	SER A	323	15.480	78 096	13.468	1.00	55.08
ATOM	2575	OG	SER A	323	14.499	77 644	12 551	1.00	52.98
ATOM	2576	C	SER A	323	16.913	78 965	11.616	1.00	54 49
ATOM	2577	O	SER A	323	18.061	78.523	11.584	1.00	58.60
ATOM	2578	N	LEU A	324	16.194	79.186	10.522	1.00	55.84
ATOM	2579	CA	LEU A	324	16.725	78.861	9.207	1.00	56.10
ATOM	2580	CB	LEU A	324	15.596	78.485	8 229	1.00	52 73
ATOM	2581	CG	LEU A	324	14.383	79.396	8.017	1.00	51.08
ATOM	2582	CD1	LEU A	324	14.679	80.431	6.945	1.00	54.72
ATOM	2583	CD2	LEU A	324	13.183	78.561	7.606	1.00	50.43
ATOM	2584	C	LEU A	324	17.637	79.928	8 625	1.00	57.85
ATOM	2585	O	LEU A	324	17.696	81.050	9.116	1.00	55.56
ATOM	2586	N	ILE A	325	18.379	79.536	7.595	1.00	62 83
ATOM	2587	CA	ILE A	325	19.307	80.428	6.910	1.00	64.52
ATOM	2588	CB	ILE A	325	20.264	79.668	5.969	1.00	64.56
ATOM	2589	CG2	ILE A	325	21.516	80.496	5.747	1.00	65.36
ATOM	2590	CG1	ILE A	325	20.591	78.271	6.516	1.00	65.53
ATOM	2591	CD1	ILE A	325	19.563	77.197	6.136	1.00	67.86
ATOM	2592	C	ILE A	325	18.501	81.383	6.034	1.00	65.56
ATOM	2593	O	ILE A	325	17.808	80.957	5.110	1.00	66 01
ATOM	2594	N	ASN A	326	18.621	82.673	6.312	1.00	67.38
ATOM	2595	CA	ASN A	326	17.899	83.696	5.559	1.00	68.33
ATOM	2596	CB	ASN A	326	18.205	85.097	6.105	1.00	73.56
ATOM	2597	CG	ASN A	326	17.632	85.325	7.495	1.00	78 94
ATOM	2598	OD1	ASN A	326	17.224	84.386	8.171	1.00	83.34
ATOM	2599	ND2	ASN A	326	17.590	86.582	7.920	1.00	79 40
ATOM	2600	C	ASN A	326	18.169	83.663	4.068	1.00	65.53
ATOM	2601	O	ASN A	326	17.254	83.861	3.274	1.00	67.11
ATOM	2602	N	LYS A	327	19.413	83.404	3.681	1.00	59 01
ATOM	2603	CA	LYS A	327	19.761	83.355	2.263	1.00	54 20
ATOM	2604	CB	LYS A	327	21.277	83.218	2.095	1.00	53 73
ATOM	2605	CG	LYS A	327	22.021	84.515	2.327	1.00	53 84
ATOM	2606	CD	LYS A	327	23.511	84.317	2.266	1.00	60.90
ATOM	2607	CE	LYS A	327	24.262	85.605	2.584	1.00	61.87
ATOM	2608	NZ	LYS A	327	24 203	86.582	1.467	1.00	58.17
ATOM	2609	C	LYS A	327	19.033	82.256	1.500	1.00	51.14
ATOM	2610	O	LYS A	327	18.610	82.472	0.370	1.00	50.58
ATOM	2611	N	ASN A	328	18.868	81.088	2.109	1.00	51.00
ATOM	2612	CA	ASN A	328	18 186	79.980	1.439	1.00	56.30
ATOM	2613	CB	ASN A	328	18 717	78.637	1.947	1.00	59.34
ATOM	2614	CG	ASN A	328	20 104	78.345	1.410	1.00	62.04
ATOM	2615	OD1	ASN A	328	21.052	79.056	1.725	1.00	64.52
ATOM	2616	ND2	ASN A	328	20 226	77.327	0.562	1.00	65.59
ATOM	2617	C	ASN A	328	16.657	80.013	1.498	1.00	56.83
ATOM	2618	O	ASN A	328	15.976	79.760	0.505	1.00	57.74
ATOM	2619	N	GLY A	329	16.117	80.291	2.684	1.00	59.02
ATOM	2620	CA	GLY A	329	14.678	80.340	2.864	1.00	57.93
ATOM	2621	C	GLY A	329	13.973	79.011	2.645	1.00	61.61
ATOM	2622	O	GLY A	329	14.604	77.939	2.645	1.00	63.66
ATOM	2623	N	GLN A	330	12.665	79.134	2.426	1.00	63.44
ATOM	2624	CA	GLN A	330	11 .647	78.088	2.186	1.00	62.51

ATOM	2625	CB	GLN	A	330	12.152	76.612	2.170	1.00	61.84
ATOM	2626	CG	GLN	A	330	11.146	75.609	1.460	1.00	62.53
ATOM	2627	CD	GLN	A	330	11.591	74.216	1.364	1.00	61.91
ATOM	2628	OE1	GLN	A	330	10.948	73.200	1.946	1.00	56.42
ATOM	2629	NE2	GLN	A	330	12.658	73.864	0.605	1.00	56.02
ATOM	2630	C	GLN	A	330	10.703	78.366	3.357	1.00	61.76
ATOM	2631	O	GLN	A	330	11.044	78.121	4.511	1.00	61.59
ATOM	2632	N	THR	A	331	9.623	79.069	3.018	1.00	61 83
ATOM	2633	CA	THR	A	331	8.542	79.549	3.891	1.00	57 39
ATOM	2634	CB	THR	A	331	8.685	79.154	5.400	1.00	46 65
ATOM	2635	OG1	THR	A	331	8.904	77.740	5.517	1.00	38 61
ATOM	2636	CG2	THR	A	331	7.378	79.483	6.144	1.00	48 69
ATOM	2637	C	THR	A	331	8.427	81.085	3.668	1.00	59 73
ATOM	2638	O	THR	A	331	8.586	81.496	2.495	1.00	55 52
ATOM	2639	OT	THR	A	331	8.131	81.869	4.601	1.00	62.34
ATOM	2640	MN	MN	A	350	10.357	71.058	3.078	1.00	32 10
ATOM	2641	MN	MN	A	351	16.765	98.946	-5.069	1.00	40.69
END										

Table 3

CRYST1	46.800	71.500	101.000	90.00	90.00	90.00			
SCALE1		0.021368	0.000000	0.000000			0.000000		
SCALE2		0.000000	0.013986	0.000000			0.000000		
SCALE3		0.000000	0.000000	0.009901			0.000000		
ATOM	1	C1	ACV	1	17.235	36.323	5.699	1.00	7.93
ATOM	2	C2	ACV	1	15.798	36.590	6 165	1.00	7.47
ATOM	3	C3	ACV	1	15 215	37.802	5 425	1.00	6.42
ATOM	4	C4	ACV	1	13.766	38.091	5 918	1.00	7.71
ATOM	5	C7	ACV	1	13 330	39 380	5.168	1.00	8.43
ATOM	6	C10	ACV	1	11 912	39.669	5 584	1.00	8.88
ATOM	7	N11	ACV	1	10.931	39.447	4 714	1.00	6.98
ATOM	8	C12	ACV	1	9 503	39.719	4 858	1.00	7.75
ATOM	9	C13	ACV	1	8 767	38.397	4.657	1.00	7 09
ATOM	10	N14	ACV	1	15 791	36 747	7 696	1.00	8.98
ATOM	11	O15	ACV	1	11 566	40.061	6 715	1.00	11.68
ATOM	12	C16	ACV	1	9.131	40 743	3.765	1.00	7.15
ATOM	13	S17	ACV	1	9 513	40.068	2.102	1.00	8 44
ATOM	14	O18	ACV	1	9.269	37.306	4 670	1.00	9.78
ATOM	15	O19	ACV	1	18 173	36.442	6.549	1.00	8.96
ATOM	16	O20	ACV	1	17.393	36.068	4.492	1.00	7.91
ATOM	17	N29	ACV	1	7.424	38.510	4.604	1.00	9.16
ATOM	18	C30	ACV	1	6.543	37 341	4.409	1.00	9 68
ATOM	19	C31	ACV	1	5.317	37.433	5 318	1.00	10 48
ATOM	20	C32	ACV	1	6 104	37 147	2.912	1 00	12 78
ATOM	21	C33	ACV	1	7 348	36 829	2 039	1.00	11.31
ATOM	22	C37	ACV	1	5 562	38 560	2 564	1.00	18.82
ATOM	23	O42	ACV	1	5 240	38.298	6.210	1.00	10.58
ATOM	24	O43	ACV	1	4.417	36.560	5 152	1.00	9.69
ATOM	25	S	SUL	2	13.002	14 100	2 417	1.00	25 69
ATOM	26	O1	SUL	2	13.804	14.598	3 492	1.00	32.83
ATOM	27	O2	SUL	2	13 918	13.558	1.424	1.00	41.91
ATOM	28	O3	SUL	2	12.155	13 073	2.934	1.00	30.42
ATOM	29	O4	SUL	2	12.299	15 076	1.614	1 00	21.23
ATOM	30	FE	IUM	1000	7.903	40 943	0 544	1.00	7.64
ATOM	31	N	SER	3	-15.013	47 966	-1.402	1.00	42.72
ATOM	32	CA	SER	3	-14.317	46 679	-1 445	1.00	39.06
ATOM	33	C	SER	3	-12 942	46.953	-2 052	1.00	36.17
ATOM	34	O	SER	3	-12 712	48.077	-2.493	1.00	41.73
ATOM	35	CB	SER	3	-14.951	45.513	-2.197	1.00	42.74
ATOM	36	OG	SER	3	-14 920	45.578	-3.613	1 00	52.50
ATOM	37	N	VAL	4	-12 127	45 917	-2.096	1.00	33.45
ATOM	38	CA	VAL	4	-10 801	46.077	-2.708	1 00	30.02
ATOM	39	C	VAL	4	-10.826	45 243	-3.983	1 00	26.11
ATOM	40	O	VAL	4	-11 331	44.137	-3.995	1.00	26 45
ATOM	41	CB	VAL	4	-9 693	45.600	-1 751	1 00	32.20
ATOM	42	CG1	VAL	4	-8 324	45 544	-2 407	1.00	31.47
ATOM	43	CG2	VAL	4	-9 619	46.380	-0 434	1.00	39.65
ATOM	44	CB	SER	5	-9.685	46.084	-7.342	1.00	28 73
ATOM	45	OG	SER	5	-10.494	46.429	-8 413	1.00	43.87
ATOM	46	C	SER	5	-9 128	43.958	-6 292	1.00	21.38
ATOM	47	O	SER	5	-8 126	44.094	-5.558	1.00	17.45
ATOM	48	N	SER	5	-10 297	45.742	-5.071	1.00	22.91
ATOM	49	CA	SER	5	-10 216	45.050	-6 347	1.00	24.13
ATOM	50	N	LYS	6	-9 338	42.900	-7 057	1.00	20 27
ATOM	51	CA	LYS	6	-8 400	41.770	-7.199	1.00	18 92
ATOM	52	CB	LYS	6	-9.148	40.516	-7 644	1.00	25.88
ATOM	53	CG	LYS	6	-8.452	39.606	-8 620	1.00	33 15
ATOM	54	CD	LYS	6	-8 676	38.116	-8 377	1.00	36 92
ATOM	55	CE	LYS	6	-9 217	37.434	-9.627	1.00	40 48
ATOM	56	NZ	LYS	6	-10.331	38.278	-10 180	1.00	49.46
ATOM	57	C	LYS	6	-7 302	42.178	-8 167	1.00	16 57
ATOM	58	O	LYS	6	-7 476	42.719	-9 294	1.00	19.33
ATOM	59	N	ALA	7	-6 060	41.933	-7.756	1.00	13 66
ATOM	60	CA	ALA	7	-4 879	42.175	-8 572	1.00	12.78
ATOM	61	CB	ALA	7	-3.616	42.083	-7 716	1.00	14.08
ATOM	62	C	ALA	7	-4.803	41.135	-9 678	1.00	12.30
ATOM	63	O	ALA	7	-5.069	39.957	-9.497	1.00	13.11
ATOM	64	N	ASN	8	-4.325	41.585	-10 844	1.00	15.13
ATOM	65	CA	ASN	8	-4.026	40.653	-11.913	1.00	16.54
ATOM	66	CB	ASN	8	-3.650	41.448	-13.197	1.00	24.27
ATOM	67	CG	ASN	8	-4.274	40.597	-14.298	1.00	29.61
ATOM	68	OD1	ASN	8	-3.669	39.640	-14.787	1.00	35.60
ATOM	69	ND2	ASN	8	-5.528	40.986	-14.477	1.00	43.75

ATOM	70	C	ASN	8	-2.738	39.882	-11.623	1.00	13.63
ATOM	71	O	ASN	8	-1.648	40.451	-11.691	1.00	16.79
ATOM	72	N	VAL	9	-2.918	38.611	-11.303	1.00	11.43
ATOM	73	CA	VAL	9	-1.809	37.707	-11.016	1.00	10.00
ATOM	74	CB	VAL	9	-1.770	37.383	-9.522	1.00	10.55
ATOM	75	CG1	VAL	9	-0.548	36.537	-9.229	1.00	10.77
ATOM	76	CG2	VAL	9	-1.726	38.675	-8.725	1 00	11.32
ATOM	77	C	VAL	9	-1 955	36.422	-11.845	1 00	10 66
ATOM	78	O	VAL	9	-2 621	35.466	-11 464	1 00	14 19
ATOM	79	N	PRO	10	-1 385	36.425	-13 059	1.00	9 44
ATOM	80	CD	PRO	10	-0 544	37.474	-13.650	1 00	10 90
ATOM	81	CA	PRO	10	-1 565	35.299	-13 942	1 00	10 48
ATOM	82	CB	PRO	10	-0.901	35.749	-15 235	1 00	12.92
ATOM	83	CG	PRO	10	-0 067	36.924	-14 937	1 00	15 89
ATOM	84	C	PRO	10	-0 883	34 026	-13 444	1 00	9 89
ATOM	85	O	PRO	10	0 125	34 091	-12 734	1 00	10.22
ATOM	86	N	LYS	11	-1 414	32 896	-13 847	1 00	9 52
ATOM	87	CA	LYS	11	-0 815	31.597	-13.586	1.00	9 53
ATOM	88	CB	LYS	11	-1.885	30.560	-13.230	1.00	12.58
ATOM	89	CG	LYS	11	-2 651	30 971	-11 965	1.00	18 45
ATOM	90	CD	LYS	11	-3 746	30.048	-11.504	1.00	23.78
ATOM	91	CE	LYS	11	-4 685	30.872	-10.629	1.00	25.46
ATOM	92	NZ	LYS	11	-4 154	31 101	-9.250	1.00	27 77
ATOM	93	C	LYS	11	0 020	31 211	-14 803	1 00	10 29
ATOM	94	O	LYS	11	-0 482	31.172	-15 926	1 00	16 95
ATOM	95	N	ILE	12	1 301	31.019	-14.640	1.00	8.18
ATOM	96	CA	ILE	12	2.214	30 697	-15 742	1 00	8 29
ATOM	97	CB	ILE	12	3.358	31 733	-15.815	1 00	8.64
ATOM	98	CG2	ILE	12	4.366	31.311	-16 864	1.00	9 33
ATOM	99	CG1	ILE	12	2 860	33 160	-16 018	1.00	9 90
ATOM	100	CD1	ILE	12	3 945	34 238	-15.984	1.00	10.28
ATOM	101	C	ILE	12	2.749	29 284	-15 518	1.00	7.89
ATOM	102	O	ILE	12	3 346	28 974	-14 504	1.00	7 80
ATOM	103	N	ASP	13	2 542	28 428	-16.522	1.00	8.72
ATOM	104	CA	ASP	13	3 109	27 068	-16.533	1 00	8 26
ATOM	105	CB	ASP	13	2 391	26 193	-17 536	1.00	9 68
ATOM	106	CG	ASP	13	2 947	24 828	-17 728	1.00	11 65
ATOM	107	OD1	ASP	13	4 047	24 478	-17 257	1 00	10.88
ATOM	108	OD2	ASP	13	2 283	24.013	-18 401	1.00	19 22
ATOM	109	C	ASP	13	4 601	27.248	-16 838	1 00	7 72
ATOM	110	O	ASP	13	5 005	27 527	-17.990	1.00	9 02
ATOM	111	N	VAL	14	5 413	26 983	-15 825	1.00	8.27
ATOM	112	CA	VAL	14	6 862	27 170	-15.947	1.00	8 27
ATOM	113	CB	VAL	14	7.453	27 766	-14 680	1 00	8 09
ATOM	114	CG1	VAL	14	6 890	29 164	-14 465	1.00	9 81
ATOM	115	CG2	VAL	14	7 298	26 882	-13 458	1 00	8.58
ATOM	116	C	VAL	14	7 592	25 910	-16.328	1.00	8.98
ATOM	117	O	VAL	14	8 815	25 950	-16.464	1 00	10 04
ATOM	118	N	SER	15	6.851	24 822	-16 531	1 00	9 65
ATOM	119	CA	SER	15	7.532	23 572	-16.883	1.00	9.94
ATOM	120	CB	SER	15	6.548	22.411	-16.994	1.00	10.80
ATOM	121	OG	SER	15	5.618	22.532	-18.063	1.00	12.34
ATOM	122	C	SER	15	8.469	23 599	-18.070	1.00	9.33
ATOM	123	O	SER	15	9 519	22 915	-18.009	1 00	9 96
ATOM	124	N	PRO	16	8 218	24 364	-19.141	1 00	10 18
ATOM	125	CD	PRO	16	7 026	25 108	-19 546	1.00	9 79
ATOM	126	CA	PRO	16	9.220	24 381	-20 209	1 00	10 12
ATOM	127	CB	PRO	16	8.629	25 357	-21.226	1 00	10 60
ATOM	128	CG	PRO	16	7.127	25 247	-21.015	1.00	11 12
ATOM	129	C	PRO	16	10 583	24 909	-19.807	1 00	9.66
ATOM	130	O	PRO	16	11.579	24.613	-20 444	1 00	11 72
ATOM	131	N	LEU	17	10 666	25 693	-18 711	1 00	10 05
ATOM	132	CA	LEU	17	11 949	26 232	-18 288	1 00	10 06
ATOM	133	CB	LEU	17	11 738	27 358	-17.276	1.00	8.52
ATOM	134	CG	LEU	17	10.992	28 598	-17.808	1 00	9.04
ATOM	135	CD1	LEU	17	10 784	29.540	-16.622	1 00	9 12
ATOM	136	CD2	LEU	17	11 738	29.314	-18.922	1 00	10 89
ATOM	137	C	LEU	17	12 890	25.183	-17 692	1 00	11 62
ATOM	138	O	LEU	17	14 087	25.442	-17 466	1 00	12 52
ATOM	139	N	PHE	18	12.403	23.970	-17.499	1.00	11.77
ATOM	140	CA	PHE	18	13.234	22.862	-17.065	1.00	12.92
ATOM	141	CB	PHE	18	12.363	21.947	-16.180	1 00	12.94
ATOM	142	CG	PHE	18	12.070	22.571	-14.820	1.00	13.53

ATOM	143	CD1	PHE	18	10 872	23.207	-14.598	1.00	17 84
ATOM	144	CD2	PHE	18	12 965	22.503	-13.766	1 00	14 00
ATOM	145	CE1	PHE	18	10 537	23 720	-13.359	1 00	17.86
ATOM	146	CE2	PHE	18	12 638	22 974	-12 519	1 00	14 38
ATOM	147	CZ	PHE	18	11 444	23.614	-12.326	1 00	15.20
ATOM	148	C	PHE	18	13.768	22.054	-18.231	1 00	14.72
ATOM	149	O	PHE	18	14.567	22 129	-18 012	1.00	17 55
ATOM	150	N	GLY	19	13.321	22.349	-19.445	1.00	15.60
ATOM	151	CA	GLY	19	13.718	21 513	-20 583	1 00	17.05
ATOM	152	C	GLY	19	14.489	22.248	-21.663	1 00	16.88
ATOM	153	O	GLY	19	15 092	23.280	-21.384	1.00	16.84
ATOM	154	N	ASP	20	14.471	21 679	-22.868	1.00	18.23
ATOM	155	CA	ASP	20	15.241	22 147	-23.997	1.00	19.57
ATOM	156	C	ASP	20	14 418	22 595	-25.186	1.00	16 96
ATOM	157	O	ASP	20	14.976	22 646	-26.285	1.00	18 78
ATOM	158	CB	ASP	20	16.172	21.025	-24.491	1.00	25.96
ATOM	159	CG	ASP	20	16.954	20.446	-23.320	1.00	30 78
ATOM	160	OD1	ASP	20	17 102	19.208	-23.399	1.00	38.92
ATOM	161	OD2	ASP	20	17 315	21 213	-22.393	1.00	40.12
ATOM	162	N	ASP	21	13 161	22.913	-25 013	1.00	16 58
ATOM	163	CA	ASP	21	12 383	23.435	-26 145	1.00	16.91
ATOM	164	CB	ASP	21	10.920	23.028	-25.985	1.00	18.23
ATOM	165	CG	ASP	21	10 023	23.362	-27.142	1.00	20.86
ATOM	166	OD1	ASP	21	10 313	24 380	-27.796	1.00	21 70
ATOM	167	OD2	ASP	21	8 968	22.756	-27.430	1.00	27 79
ATOM	168	C	ASP	21	12 561	24.961	-26.116	1.00	14.20
ATOM	169	O	ASP	21	11.892	25.648	-25.343	1.00	12.84
ATOM	170	N	GLN	22	13.504	25.500	-26.887	1.00	15 68
ATOM	171	CA	GLN	22	13 813	26.915	-26.764	1.00	13.82
ATOM	172	CB	GLN	22	15.048	27.347	-27.545	1.00	13 58
ATOM	173	CG	GLN	22	16.257	26.474	-27.348	1.00	15.37
ATOM	174	CD	GLN	22	16.663	26 189	-25.918	1.00	16.56
ATOM	175	OE1	GLN	22	16.485	27 042	-25.067	1.00	19.01
ATOM	176	NE2	GLN	22	17 205	24.984	-25.728	1.00	19 39
ATOM	177	C	GLN	22	12.654	27.819	-27.116	1.00	13 52
ATOM	178	O	GLN	22	12.484	28.853	-26.449	1.00	11.96
ATOM	179	N	ALA	23	11.890	27.480	-28.125	1.00	16.53
ATOM	180	CA	ALA	23	10.739	28.320	-28.488	1.00	16.41
ATOM	181	CB	ALA	23	10.088	27.855	-29.796	1.00	22.56
ATOM	182	C	ALA	23	9.715	28.331	-27.352	1.00	13.99
ATOM	183	O	ALA	23	9 120	29.380	-27.065	1.00	13.68
ATOM	184	N	ALA	24	9 451	27.160	-26.761	1.00	13 08
ATOM	185	CA	ALA	24	8 481	27.122	-25.650	1 00	11 55
ATOM	186	CB	ALA	24	8 214	25.694	-25.217	1.00	13.62
ATOM	187	C	ALA	24	8.988	27.977	-24.524	1 00	9.62
ATOM	188	O	ALA	24	8 213	28 627	-23.815	1.00	9.80
ATOM	189	N	LYS	25	10 278	27 958	-24.263	1 00	10.01
ATOM	190	CA	LYS	25	10 844	28 781	-23.178	1 00	9.16
ATOM	191	CB	LYS	25	12 332	28.472	-23.004	1 00	9 87
ATOM	192	CG	LYS	25	12.600	27.128	-22.327	1.00	13.94
ATOM	193	CD	LYS	25	14 077	27.106	-21.852	1.00	21.25
ATOM	194	CE	LYS	25	14.817	25 974	-22 406	1.00	24.07
ATOM	195	NZ	LYS	25	16 254	26 073	-22 150	1 00	19.05
ATOM	196	C	LYS	25	10 657	30.249	-23.474	1 00	7.92
ATOM	197	O	LYS	25	10.375	31.042	-22 566	1.00	8.19
ATOM	198	N	MET	26	10 811	30.662	-24 728	1 00	8.75
ATOM	199	CA	MET	26	10 564	32.085	-25.068	1.00	9.12
ATOM	200	CB	MET	26	10.903	32 408	-26 546	1 00	9.73
ATOM	201	CG	MET	26	12.399	32.424	-26.816	1 00	10.03
ATOM	202	SD	MET	26	13.322	33.724	-25 970	1 00	10.21
ATOM	203	CE	MET	26	13.056	35.132	-27.066	1.00	10.95
ATOM	204	C	MET	26	9 115	32 487	-24 804	1 00	8 72
ATOM	205	O	MET	26	8.828	33.594	-24 356	1 00	8.27
ATOM	206	N	ARG	27	8.163	31 585	-25 091	1.00	8 42
ATOM	207	CA	ARG	27	6.767	31 903	-24.809	1 00	9.14
ATOM	208	CB	ARG	27	5.842	30 894	-25.505	1 00	10 27
ATOM	209	CG	ARG	27	5.895	31 042	-27.031	1 00	11.63
ATOM	210	CD	ARG	27	4.969	30 149	-27.808	1 00	15.41
ATOM	211	NE	ARG	27	5.322	28.732	-27.657	1 00	17.68
ATOM	212	CZ	ARG	27	5.998	28 016	-28.551	1 00	17.12
ATOM	213	NH1	ARG	27	6.271	26 720	-28.347	1 00	18.08
ATOM	214	NH2	ARG	27	6.357	28 591	-29.680	1 00	19.32
ATOM	215	C	ARG	27	6.496	32 020	-23.319	1.00	9.48

ATOM	216	O	ARG	27	5.649	32.854	-22.925	1.00	9.79
ATOM	217	N	VAL	28	7.214	31.249	-22.488	1.00	7.80
ATOM	218	CA	VAL	28	7.129	31.447	-21.039	1.00	7.60
ATOM	219	CB	VAL	28	7.799	30.307	-20.275	1.00	8.02
ATOM	220	CG1	VAL	28	7.803	30.582	-18.782	1.00	9.37
ATOM	221	CG2	VAL	28	7.194	28.970	-20.553	1.00	10.98
ATOM	222	C	VAL	28	7.743	32.786	-20.643	1.00	7.31
ATOM	223	O	VAL	28	7.164	33.556	-19.853	1.00	7.76
ATOM	224	N	ALA	29	8.909	33.096	-21.235	1.00	7 04
ATOM	225	CA	ALA	29	9.578	34.368	-20.949	1.00	7.37
ATOM	226	CB	ALA	29	10 870	34.447	-21.743	1.00	7 98
ATOM	227	C	ALA	29	8 691	35.579	-21.233	1.00	7 31
ATOM	228	O	ALA	29	8.662	36.547	-20 478	1.00	8 13
ATOM	229	N	GLN	30	7 902	35.483	-22.319	1.00	7 11
ATOM	230	CA	GLN	30	7 001	36 576	-22 637	1.00	7 56
ATOM	231	CB	GLN	30	6 261	36.323	-23.976	1.00	8.19
ATOM	232	CG	GLN	30	5 378	37 456	-24 427	1.00	8 58
ATOM	233	CD	GLN	30	3.966	37 535	-23 845	1.00	8 95
ATOM	**234**	**OE1**	**GLN**	**30**	**3.396**	**36.491**	**-23.534**	**1.00**	**10.78**
ATOM	235	NE2	GLN	30	3 570	38 741	-23.481	1.00	9.99
ATOM	236	C	GLN	30	6 005	36.784	-21.497	1.00	6 94
ATOM	237	O	GLN	30	5 631	37 936	-21.231	1.00	8 27
ATOM	238	N	GLN	31	5.464	35 677	-20 996	1.00	7 41
ATOM	239	CA	GLN	31	4 470	35 750	-19 933	1.00	7 30
ATOM	240	CB	GLN	31	3.924	34 357	-19 675	1 00	8.13
ATOM	241	CG	GLN	31	3.117	33 748	-20.829	1.00	9.37
ATOM	242	CD	GLN	31	2.722	32 316	-20.493	1.00	11 83
ATOM	243	OE1	GLN	31	1.843	32 090	-19.656	1.00	15 21
ATOM	244	NE2	GLN	31	3.391	31 367	-21.108	1.00	18 42
ATOM	245	C	GLN	31	5.093	36 370	-18 681	1.00	7 43
ATOM	246	O	GLN	31	4 459	37 197	-18 024	1 00	7.98
ATOM	247	N	ILE	32	6 326	36.030	-18.367	1 00	6 96
ATOM	248	CA	ILE	32	7 047	36.640	-17 258	1 00	7.29
ATOM	249	CB	ILE	32	8.389	35 925	-17 010	1 00	7 37
ATOM	250	CG2	ILE	32	9.254	36.685	-16.004	1 00	9 11
ATOM	251	CG1	ILE	32	8 126	34 504	-16.497	1.00	7.84
ATOM	252	CD1	ILE	32	9.335	33 611	-16.390	1 00	9.10
ATOM	253	C	ILE	32	7 235	38 139	-17 496	1.00	7.13
ATOM	254	O	ILE	32	7.023	38.945	-16 602	1.00	8 31
ATOM	255	N	ASP	33	7.632	38 515	-18 717	1 00	7 76
ATOM	256	CA	ASP	33	7.801	39 927	-19 072	1 00	8 04
ATOM	257	CB	ASP	33	8.257	40 026	-20 550	1.00	8.19
ATOM	258	CG	ASP	33	8.447	41 482	-20 994	1 00	8.88
ATOM	259	OD1	ASP	33	9 429	42 118	-20.550	1 00	9 63
ATOM	260	OD2	ASP	33	7 560	41 941	-21 792	1 00	9 07
ATOM	261	C	ASP	33	6 480	40 675	-18 835	1 00	7.95
ATOM	262	O	ASP	33	6.480	41 751	-18.200	1 00	8 54
ATOM	263	N	ALA	34	5.357	40 154	-19.355	1 00	8 10
ATOM	264	CA	ALA	34	4.079	40.834	-19.202	1 00	8.69
ATOM	265	CB	ALA	34	2.993	40 062	-19 938	1 00	9 24
ATOM	266	C	ALA	34	3.709	41 028	-17.735	1.00	8.36
ATOM	267	O	ALA	34	3.284	42.105	-17 299	1.00	9 82
ATOM	268	N	ALA	35	3.903	39.967	-16 933	1 00	8.64
ATOM	269	CA	ALA	35	3 505	40.093	-15 538	1 00	9.10
ATOM	270	CB	ALA	35	3.527	38 723	-14 870	1 00	11.05
ATOM	271	C	ALA	35	4 423	41 047	-14 779	1 00	9.17
ATOM	272	O	ALA	35	3 968	41 822	-13.942	1.00	10 62
ATOM	273	N	SER	36	5.709	41.042	-15 146	1.00	8.20
ATOM	274	CA	SER	36	6 683	41 896	-14.467	1.00	7.99
ATOM	275	CB	SER	36	8.108	41 485	-14.830	1.00	8 90
ATOM	276	OG	SER	36	8 354	40 129	-14.485	1 00	8.75
ATOM	277	C	SER	36	6 436	43 364	-14.801	1.00	9 43
ATOM	278	O	SER	36	6 761	44 224	-13.994	1.00	12 45
ATOM	279	N	ARG	37	5 871	43 633	-15.993	1.00	9.00
ATOM	280	CA	ARG	37	5 572	44 996	-16.415	1.00	10 53
ATOM	281	CB	ARG	37	5 685	45 095	-17.931	1.00	11 22
ATOM	282	CG	ARG	37	7 046	44 858	-18.544	1.00	12 00
ATOM	283	CD	ARG	37	7 074	44 615	-20.051	1.00	14 37
ATOM	284	NE	ARG	37	6 514	45.706	-20.881	1.00	15 54
ATOM	285	CZ	ARG	37	6.327	45.575	-22.190	1.00	15 00
ATOM	286	NH1	ARG	37	6.682	44.430	-22.781	1.00	16 31
ATOM	287	NH2	ARG	37	5 812	46.595	-22.875	1.00	14 97
ATOM	288	C	ARG	37	4.204	45.459	-15.925	1.00	11.82

ATOM	289	O	ARG	37	3.914	46.654	-15 947	1 00	17 60
ATOM	290	N	ASP	38	3.367	44.520	-15 475	1.00	12.19
ATOM	291	CA	ASP	38	2 045	44.889	-14 976	1 00	14 66
ATOM	292	CB	ASP	38	1 017	43.860	-15.463	1 00	16.65
ATOM	293	CG	ASP	38	-0 441	44.105	-15 173	1 00	17.06
ATOM	294	OD1	ASP	38	-0 763	45.278	-14 922	1.00	22 39
ATOM	295	OD2	ASP	38	-1 316	43.219	-15.263	1 00	20 09
ATOM	296	C	ASP	38	2 102	45.018	-13 455	1 00	13 71
ATOM	297	O	ASP	38	2 736	45.927	-12.904	1.00	14 27
ATOM	298	N	THR	39	1 460	44.073	-12 737	1 00	11 56
ATOM	299	CA	THR	39	1 415	44.205	-11.298	1 00	11.81
ATOM	300	CB	THR	39	0.320	43.390	-10 584	1 00	14.06
ATOM	301	OG1	THR	39	0.687	41.990	-10 698	1.00	17.03
ATOM	302	CG2	THR	39	-1 008	43.691	-11 223	1 00	17 60
ATOM	303	C	THR	39	2.721	43 776	-10 634	1 00	10.17
ATOM	304	O	THR	39	2.920	44.118	-9.459	1.00	11.25
ATOM	305	N	GLY	40	3.510	42.982	-11.367	1.00	9.14
ATOM	306	CA	GLY	40	4 740	42.526	-10 777	1 00	8.52
ATOM	307	C	GLY	40	4.618	41.278	-10 115	1.00	9.63
ATOM	308	O	GLY	40	5.587	40.753	-9 505	1.00	14.89
ATOM	309	N	PHE	41	3 477	40.522	-10 124	1.00	8.18
ATOM	310	CA	PHE	41	3.307	39.207	-9 532	1.00	7 48
ATOM	311	CB	PHE	41	2.353	39.290	-8 343	1.00	7 50
ATOM	312	CG	PHE	41	2.952	39.927	-7 078	1.00	7 93
ATOM	313	CD1	PHE	41	2.936	41.286	-6.859	1.00	8 43
ATOM	314	CD2	PHE	41	3 499	39.110	-6.100	1.00	7 47
ATOM	315	CE1	PHE	41	3.446	41.812	-5.683	1.00	8.79
ATOM	316	CE2	PHE	41	4.040	39 635	-4 933	1.00	8.21
ATOM	317	CZ	PHE	41	4.032	40 998	-4 757	1.00	8 46
ATOM	318	C	PHE	41	2.782	38.226	-10 550	1.00	6 88
ATOM	319	O	PHE	41	1.952	38.554	-11 401	1.00	9.03
ATOM	320	N	PHE	42	3.164	36.978	-10.374	1.00	6.68
ATOM	321	CA	PHE	42	2.539	35.845	-11.075	1.00	6.92
ATOM	322	CB	PHE	42	3 148	35.586	-12.456	1.00	7.96
ATOM	323	CG	PHE	42	4.564	35.072	-12.516	1.00	7.35
ATOM	324	CD1	PHE	42	4.802	33 699	-12.586	1.00	7.79
ATOM	325	CD2	PHE	42	5.637	35.931	-12 518	1 00	8.85
ATOM	326	CE1	PHE	42	6.124	33.266	-12.696	1.00	8 64
ATOM	327	CE2	PHE	42	6 951	35.498	-12 656	1.00	9.37
ATOM	328	CZ	PHE	42	7 193	34 141	-12.740	1.00	9.28
ATOM	329	C	PHE	42	2.620	34.594	-10.216	1 00	6.60
ATOM	330	O	PHE	42	3 489	34.518	-9.338	1.00	6 98
ATOM	331	N	TYR	43	1 783	33 606	-10 477	1 00	6.57
ATOM	332	CA	TYR	43	1 913	32.290	-9.860	1 00	6.96
ATOM	333	CB	TYR	43	0 575	31 694	-9 466	1 00	7.72
ATOM	334	CG	TYR	43	0.098	32 111	-8 088	1 00	7 41
ATOM	335	CD1	TYR	43	-0 901	33 078	-7 938	1 00	8 92
ATOM	336	CE1	TYR	43	-1 335	33.480	-6.697	1.00	9.19
ATOM	337	CD2	TYR	43	0 664	31.618	-6 939	1 00	7 76
ATOM	338	CE2	TYR	43	0.248	32.035	-5 690	1 00	8 82
ATOM	339	CZ	TYR	43	-0 715	32 992	-5 574	1.00	9 99
ATOM	340	OH	TYR	43	-1.130	33 349	-4 303	1.00	11 00
ATOM	341	C	TYR	43	2.625	31.390	-10.867	1.00	6 77
ATOM	342	O	TYR	43	2.160	31.203	-11.985	1 00	9.17
ATOM	343	N	ALA	44	3 663	30.736	-10 386	1 00	6.74
ATOM	344	CA	ALA	44	4.321	29.654	-11.138	1.00	6.80
ATOM	345	CB	ALA	44	5.766	29.522	-10 683	1 00	6.89
ATOM	346	C	ALA	44	3 590	28.345	-10.834	1 00	6.81
ATOM	347	O	ALA	44	3.423	27.965	-9.679	1.00	7.69
ATOM	348	N	VAL	45	3 075	27.695	-11 849	1 00	7.45
ATOM	349	CA	VAL	45	2 373	26.431	-11 766	1.00	7.41
ATOM	350	CB	VAL	45	0 902	26.570	-12.161	1 00	9.68
ATOM	351	CG1	VAL	45	0.228	27.601	-11 255	1.00	10.94
ATOM	352	CG2	VAL	45	0.670	26.895	-13 632	1.00	10.29
ATOM	353	C	VAL	45	3.120	25.384	-12.583	1 00	7.22
ATOM	354	O	VAL	45	3.984	25.718	-13.393	1.00	7.51
ATOM	355	N	ASN	46	2.862	24.095	-12.325	1.00	8.30
ATOM	356	CA	ASN	46	3.565	22.985	-12.948	1.00	8.32
ATOM	357	CB	ASN	46	3.323	22.885	-14.449	1.00	11.81
ATOM	358	CG	ASN	46	1.875	22.704	-14.786	1.00	18.20
ATOM	359	OD1	ASN	46	1.395	21.610	-14.470	1.00	31.96
ATOM	360	ND2	ASN	46	1.269	23.750	-15.306	1.00	24.56
ATOM	361	C	ASN	46	5.043	23.111	-12.634	1.00	8.17

ATOM	362	O	ASN	46	5.936	22.860	-13.449	1.00	10.28
ATOM	363	N	HIS	47	5.323	23.425	-11.366	1.00	8.42
ATOM	364	CA	HIS	47	6.663	23.646	-10.843	1.00	8.14
ATOM	365	CB	HIS	47	6.618	24.724	-9.775	1.00	8.35
ATOM	366	CG	HIS	47	5.590	24 430	-8.727	1.00	7 34
ATOM	367	CD2	HIS	47	4.399	25 000	-8.504	1.00	7 88
ATOM	368	ND1	HIS	47	5.719	23 383	-7.812	1.00	7 39
ATOM	369	CE1	HIS	47	4.626	23 360	-7.052	1.00	8 04
ATOM	370	NE2	HIS	47	3.827	24 344	-7.440	1.00	8 14
ATOM	371	C	HIS	47	7.375	22 430	-10.325	1.00	7 89
ATOM	372	O	HIS	47	8.580	22 464	-10.091	1.00	9 85
ATOM	373	N	GLY	48	6.691	21 328	-10.139	1.00	8 33
ATOM	374	CA	GLY	48	7.238	20.053	-9.749	1.00	8 83
ATOM	375	C	GLY	48	7.522	19 849	-8.282	1.00	8 46
ATOM	376	O	GLY	48	8.060	18 780	-7.953	1 00	11.24
ATOM	377	N	ILE	49	7.267	20 817	-7.412	1 00	7.06
ATOM	378	CA	ILE	49	7.568	20 636	-6.015	1.00	6 70
ATOM	379	CB	ILE	49	8.093	21.962	-5.389	1.00	7.04
ATOM	**380**	**CG2**	**ILE**	**49**	**8.286**	**21.829**	**-3.886**	**1.00**	**7.67**
ATOM	381	CG1	ILE	49	9.383	22.383	-6 077	1 00	8.13
ATOM	382	CD1	ILE	49	9 964	23 699	-5.584	1.00	9.61
ATOM	383	C	ILE	49	6 327	20.166	-5 245	1.00	6.55
ATOM	384	O	ILE	49	5.210	20 605	-5.497	1 00	7 34
ATOM	385	N	ASN	50	6 531	19 246	-4.311	1 00	6.14
ATOM	386	CA	ASN	50	5 449	18 729	-3.464	1 00	5 89
ATOM	387	CB	ASN	50	5 834	17.332	-2 967	1.00	6 25
ATOM	388	CG	ASN	50	4 688	16 658	-2.270	1 00	5.80
ATOM	389	OD1	ASN	50	3.717	17.297	-1.870	1.00	7.60
ATOM	390	ND2	ASN	50	4 840	15.366	-2 058	1.00	7 26
ATOM	391	C	ASN	50	5 184	19 714	-2 331	1 00	5 68
ATOM	392	O	ASN	50	5.744	19.597	-1.230	1.00	6.62
ATOM	393	N	VAL	51	4 328	20.676	-2.619	1.00	5.97
ATOM	394	CA	VAL	51	4 037	21.706	-1.632	1.00	6.10
ATOM	395	CB	VAL	51	3.508	23 010	-2 290	1.00	6 74
ATOM	396	CG1	VAL	51	4 557	23 676	-3 184	1.00	9 06
ATOM	397	CG2	VAL	51	2 250	22.743	-3.048	1.00	9 15
ATOM	398	C	VAL	51	3.137	21.232	-0 504	1 00	7.22
ATOM	399	O	VAL	51	3.299	21.758	0 610	1.00	7 84
ATOM	400	N	GLN	52	2 286	20.231	-0.761	1 00	7 44
ATOM	401	CA	GLN	52	1 474	19 721	0 339	1 00	6 88
ATOM	402	CB	GLN	52	0 442	18 728	-0 163	1 00	8 70
ATOM	403	CG	GLN	52	-0 534	18 205	0 917	1.00	10 71
ATOM	404	CD	GLN	52	-0 066	17 059	1 807	1.00	12 39
ATOM	405	OE1	GLN	52	0.970	16 387	1 579	1.00	12.25
ATOM	406	NE2	GLN	52	-0 672	16 925	2.956	1 00	13.45
ATOM	407	C	GLN	52	2.410	19 094	1 378	1.00	6 81
ATOM	408	O	GLN	52	2 162	19.264	2.599	1 00	6 97
ATOM	409	N	ARG	53	3.434	18.364	0 950	1 00	6.70
ATOM	410	CA	ARG	53	4.339	17 734	1 912	1.00	6.00
ATOM	411	CB	ARG	53	5.152	16 655	1 210	1.00	6.55
ATOM	412	CG	ARG	53	6.068	15 894	2.129	1.00	6 59
ATOM	413	CD	ARG	53	6.645	14.676	1 432	1.00	8.72
ATOM	414	NE	ARG	53	7.445	13 846	2 348	1.00	8.70
ATOM	415	CZ	ARG	53	8 771	13 910	2 425	1.00	10.05
ATOM	416	NH1	ARG	53	9 464	14 723	1 605	1.00	12 80
ATOM	417	NH2	ARG	53	9 424	13 106	3.279	1 00	10.00
ATOM	418	C	ARG	53	5 156	18.809	2 598	1.00	5.84
ATOM	419	O	ARG	53	5 396	18 698	3 820	1.00	6 89
ATOM	420	N	LEU	54	5 598	19 850	1.903	1.00	5.98
ATOM	421	CA	LEU	54	6 274	20 982	2 544	1 00	5 87
ATOM	422	CB	LEU	54	6 558	22 056	1 489	1.00	6 27
ATOM	423	CG	LEU	54	6 940	23 435	2 017	1 00	7.00
ATOM	424	CD1	LEU	54	8 286	23 396	2 689	1 00	7.98
ATOM	425	CD2	LEU	54	6 864	24.441	0 866	1 00	8.66
ATOM	426	C	LEU	54	5 406	21 576	3 660	1 00	5.97
ATOM	427	O	LEU	54	5 870	21 822	4 788	1 00	6.89
ATOM	428	N	SER	55	4 136	22.786	3 344	1.00	6.27
ATOM	429	CA	SER	55	3 240	22.335	4 357	1 00	6.86
ATOM	430	CB	SER	55	1 916	22.675	3 694	1 00	7.85
ATOM	431	OG	SER	55	0.981	23.194	4 615	1 00	11.52
ATOM	432	C	SER	55	3.098	21.410	5 563	1 00	6.98
ATOM	433	O	SER	55	3.081	21.834	6.713	1.00	7.09
ATOM	434	N	GLN	56	2.961	20.107	5.309	1.00	7.22

ATOM	435	CA	GLN	56	2.784	19.139	6.379	1.00	7.20
ATOM	436	CB	GLN	56	2.400	17.785	5 799	1.00	9.23
ATOM	437	CG	GLN	56	2.329	16.657	6.795	1.00	11.52
ATOM	438	CD	GLN	56	1.214	16.804	7 803	1.00	14.79
ATOM	439	OE1	GLN	56	1 405	16.302	8.912	1.00	22.67
ATOM	440	NE2	GLN	56	0 122	17.443	7 423	1.00	13.58
ATOM	441	C	GLN	56	4.007	19.101	7 279	1.00	7.77
ATOM	442	O	GLN	56	3.869	19.099	8.517	1.00	7.98
ATOM	443	N	LYS	57	5.188	18.978	6 684	1.00	6.97
ATOM	444	CA	LYS	57	6.404	18.904	7 465	1.00	7.11
ATOM	445	CB	LYS	57	7 622	18.583	6 598	1.00	7.89
ATOM	446	CG	LYS	57	7 574	17.249	5.861	1.00	7.92
ATOM	447	CD	LYS	57	7 561	16.023	6 784	1.00	9 42
ATOM	448	CE	LYS	57	7 650	14.765	5.962	1.00	10 57
ATOM	449	NZ	LYS	57	7 444	13.524	6.770	1.00	13.31
ATOM	450	C	LYS	57	6 623	20.175	8.273	1.00	6 73
ATOM	451	O	LYS	57	7.102	20.149	9.413	1.00	8.29
ATOM	452	N	THR	58	6.325	21.322	7.676	1.00	7.11
ATOM	453	CA	THR	58	6 448	22.618	8.342	1.00	7 21
ATOM	454	CB	THR	58	6 257	23.767	7.355	1.00	7.45
ATOM	455	OG1	THR	58	7 318	23.725	6.392	1.00	8.22
ATOM	456	CG2	THR	58	6.316	25.134	8.054	1.00	8.05
ATOM	457	C	THR	58	5.495	22.727	9.527	1.00	6.99
ATOM	458	O	THR	58	5 879	23.194	10.618	1.00	7.76
ATOM	459	N	LYS	59	4.257	22.255	9.336	1.00	7.98
ATOM	460	CA	LYS	59	3 270	22.244	10.430	1.00	8 41
ATOM	461	CB	LYS	59	1 933	21.732	9.870	1.00	11.31
ATOM	462	CG	LYS	59	0.857	21.678	10.962	1.00	17.36
ATOM	463	CD	LYS	59	-0.412	21.032	10.378	1.00	21.57
ATOM	464	CE	LYS	59	-0.145	19.572	10.080	1.00	26.63
ATOM	465	NZ	LYS	59	0.949	19.018	10.953	1.00	41.28
ATOM	466	C	LYS	59	3.756	21.375	11.583	1.00	8.97
ATOM	467	O	LYS	59	3.662	21.789	12.743	1.00	9.25
ATOM	468	N	GLU	60	4.260	20.182	11.254	1.00	8.73
ATOM	469	CA	GLU	60	4.763	19.297	12.288	1.00	9.20
ATOM	470	CB	GLU	60	5.286	17.988	11.679	1.00	10.60
ATOM	471	CG	GLU	60	4.189	17.114	11.083	1.00	13.69
ATOM	472	CD	GLU	60	4.634	15.954	10.241	1.00	15.34
ATOM	473	OE1	GLU	60	5.846	15.700	10.211	1.00	20.83
ATOM	474	OE2	GLU	60	3.819	15.290	9.550	1.00	19.42
ATOM	475	C	GLU	60	5.849	19.961	13.119	1.00	10 04
ATOM	476	O	GLU	60	5.822	19.898	14.353	1.00	11.42
ATOM	477	N	PHE	61	6.751	20.687	12.465	1.00	8.91
ATOM	478	CA	PHE	61	7.785	21.443	13.184	1.00	7.35
ATOM	479	CB	PHE	61	8.775	21.958	12.129	1.00	7.73
ATOM	480	CG	PHE	61	9.763	22.977	12.665	1.00	8 40
ATOM	481	CD1	PHE	61	10.749	22.594	13.521	1.00	9.42
ATOM	482	CD2	PHE	61	9.667	24.316	12.302	1.00	10.73
ATOM	483	CE1	PHE	61	11.653	23.520	13.994	1.00	10.45
ATOM	484	CE2	PHE	61	10.591	25.256	12.727	1.00	11 37
ATOM	485	CZ	PHE	61	11.562	24.834	13.606	1.00	10.57
ATOM	486	C	PHE	61	7.211	22.579	14.015	1.00	7.60
ATOM	487	O	PHE	61	7.474	22.658	15.228	1.00	8.53
ATOM	488	N	HIS	62	6.446	23.487	13.426	1.00	8 25
ATOM	489	CA	HIS	62	5.921	24.635	14.156	1.00	8.66
ATOM	490	CB	HIS	62	5.076	25.531	13.261	1.00	9.03
ATOM	491	CG	HIS	62	5.800	26.423	12.311	1.00	8 36
ATOM	492	CD2	HIS	62	5.271	26 774	11 094	1.00	7 90
ATOM	493	ND1	HIS	62	6.963	27 124	12.415	1.00	10.22
ATOM	494	CE1	HIS	62	7.123	27.845	11.303	1 00	7 76
ATOM	495	NE2	HIS	62	6.122	27.622	10 488	1 00	10 59
ATOM	496	C	HIS	62	5.091	24 264	15 385	1.00	9.71
ATOM	497	O	HIS	62	5.070	24.974	16.376	1 00	11 19
ATOM	498	N	MET	63	4.335	23 167	15 283	1 00	10 41
ATOM	499	CA	MET	63	3.393	22 836	16 321	1 00	12.27
ATOM	500	CB	MET	63	2.151	22 162	15.705	1 00	13 32
ATOM	501	CG	MET	63	1.453	23.061	14.692	1 00	14.13
ATOM	502	SD	MET	63	1.062	24.757	15.253	1.00	21.44
ATOM	503	CE	MET	63	0.528	25.519	13.715	1.00	41.15
ATOM	504	C	MET	63	4.020	22.008	17.416	1.00	13.21
ATOM	505	O	MET	63	3.383	21.818	18.470	1.00	19.62
ATOM	506	N	SER	64	5.203	21.457	17.178	1.00	10.61
ATOM	507	CA	SER	64	5.896	20.662	18.191	1.00	13.44

ATOM	508	CB	SER	64	6.289	19.283	17.662	1.00	15.79
ATOM	509	OG	SER	64	7.299	19.356	16.689	1.00	17.37
ATOM	510	C	SER	64	7.105	21.342	18.809	1.00	12.71
ATOM	511	O	SER	64	7.528	20.933	19.888	1.00	16.31
ATOM	512	N	ILE	65	7.664	22.392	18.236	1.00	10.13
ATOM	513	CA	ILE	65	8.799	23.010	18.900	1.00	9.79
ATOM	514	CB	ILE	65	9.469	23.968	17.906	1.00	10.92
ATOM	515	CG2	ILE	65	8.583	25.072	17.406	1.00	13.10
ATOM	516	CG1	ILE	65	10.787	24.455	18.502	1.00	11.85
ATOM	517	CD1	ILE	65	11.740	25.156	17.598	1.00	13.44
ATOM	518	C	ILE	65	8.366	23.703	20.162	1.00	10.18
ATOM	519	O	ILE	65	7.286	24.267	20.263	1.00	12.62
ATOM	520	N	THR	66	9.170	23.608	21.194	1.00	10.22
ATOM	521	CA	THR	66	8.866	24.106	22.535	1.00	10.06
ATOM	522	CB	THR	66	9.278	23.065	23.583	1.00	9.97
ATOM	523	OG1	THR	66	10.681	22.892	23.511	1.00	12.07
ATOM	524	CG2	THR	66	8.571	22.749	23.373	1.00	14.54
ATOM	525	C	THR	66	9.559	25.420	22.846	1.00	8.74
ATOM	526	O	THR	66	10.531	25.775	22.160	1.00	8.66
ATOM	527	N	PRO	67	9.078	26.142	23.864	1.00	9.12
ATOM	528	CD	PRO	67	7.813	25.938	24.594	1.00	11.31
ATOM	529	CA	PRO	67	9.724	27.392	24.251	1.00	9.65
ATOM	530	CB	PRO	67	8.925	27.860	25.450	1.00	12.19
ATOM	531	CG	PRO	67	7.598	27.233	25.312	1.00	12.99
ATOM	532	C	PRO	67	11.209	27.228	24.567	1.00	9.34
ATOM	533	O	PRO	67	12.046	28.064	24.200	1.00	10.59
ATOM	534	N	GLU	68	11.597	26.115	25.186	1.00	10.47
ATOM	535	CA	GLU	68	13.000	25.861	25.470	1.00	11.64
ATOM	536	CB	GLU	68	13.061	24.533	26.244	1.00	13.13
ATOM	537	CG	GLU	68	14.452	24.123	26.600	1.00	14.22
ATOM	538	CD	GLU	68	14.498	22.689	27.107	1.00	15.39
ATOM	539	OE1	GLU	68	13.945	22.743	26.508	1.00	21.02
ATOM	540	OE2	GLU	68	15.043	22.449	28.180	1.00	19.65
ATOM	541	C	GLU	68	13.836	25.799	24.217	1.00	9.32
ATOM	542	O	GLU	68	14.920	26.376	24.096	1.00	11.18
ATOM	543	N	GLU	69	13.319	25.065	23.221	1.00	8.89
ATOM	544	CA	GLU	69	14.015	24.920	21.929	1.00	9.17
ATOM	545	CB	GLU	69	13.310	23.921	21.010	1.00	9.44
ATOM	546	CG	GLU	69	13.338	22.513	21.576	1.00	10.83
ATOM	547	CD	GLU	69	12.432	21.627	20.745	1.00	12.92
ATOM	548	OE1	GLU	69	12.996	20.941	19.876	1.00	19.22
ATOM	549	OE2	GLU	69	11.213	21.599	21.003	1.00	19.62
ATOM	550	C	GLU	69	14.157	26.247	21.213	1.00	8.87
ATOM	551	O	GLU	69	15.153	26.521	20.573	1.00	9.17
ATOM	552	N	LYS	70	13.126	27.086	21.311	1.00	8.65
ATOM	553	CA	LYS	70	13.148	28.387	20.621	1.00	8.41
ATOM	554	CB	LYS	70	11.786	29.100	20.695	1.00	8.73
ATOM	555	CG	LYS	70	10.663	29.358	19.977	1.00	8.40
ATOM	556	CD	LYS	70	9.319	29.001	20.239	1.00	9.16
ATOM	557	CE	LYS	70	8.198	28.102	19.726	1.00	10.86
ATOM	558	NZ	LYS	70	6.875	28.741	19.900	1.00	12.00
ATOM	559	C	LYS	70	14.268	29.257	21.182	1.00	7.77
ATOM	560	O	LYS	70	14.992	29.885	20.400	1.00	8.10
ATOM	561	N	TRP	71	14.418	29.325	22.514	1.00	7.55
ATOM	562	CA	TRP	71	15.556	30.080	23.057	1.00	7.86
ATOM	563	CB	TRP	71	15.545	30.104	24.582	1.00	8.53
ATOM	564	CG	TRP	71	14.467	30.932	25.195	1.00	7.80
ATOM	565	CD2	TRP	71	14.216	32.335	25.045	1.00	7.55
ATOM	566	CE2	TRP	71	13.097	32.672	25.824	1.00	8.56
ATOM	567	CE3	TRP	71	14.813	33.362	24.326	1.00	8.26
ATOM	568	CD1	TRP	71	13.512	30.477	26.068	1.00	8.54
ATOM	569	NE1	TRP	71	12.682	31.521	26.446	1.00	9.24
ATOM	570	CZ2	TRP	71	12.589	33.965	25.900	1.00	9.23
ATOM	571	CZ3	TRP	71	14.311	34.644	24.384	1.00	8.95
ATOM	572	CH2	TRP	71	13.198	34.947	25.181	1.00	9.37
ATOM	573	C	TRP	71	16.892	29.513	22.565	1.00	7.41
ATOM	574	O	TRP	71	17.808	30.271	22.223	1.00	7.75
ATOM	575	N	ASP	72	16.954	28.180	22.552	1.00	7.95
ATOM	576	CA	ASP	72	18.195	27.508	22.215	1.00	9.24
ATOM	577	CB	ASP	72	18.123	26.031	22.638	1.00	11.24
ATOM	578	CG	ASP	72	18.208	25.822	24.146	1.00	14.08
ATOM	579	OD1	ASP	72	18.351	26.778	24.967	1.00	15.23
ATOM	580	OD2	ASP	72	17.942	24.678	24.599	1.00	17.93

ATOM	581	C	ASP	72	18.589	27 715	20.764	1.00	9 14
ATOM	582	O	ASP	72	19.766	27 648	20.413	1.00	10 16
ATOM	583	N	LEU	73	17 615	27 980	19.872	1.00	7 62
ATOM	584	CA	LEU	73	17 828	28 233	18.474	1.00	8.24
ATOM	585	CB	LEU	73	16 767	27 452	17.648	1.00	9 44
ATOM	586	CG	LEU	73	16.895	25.941	17.683	1.00	10.93
ATOM	587	CD1	LEU	73	15 676	25 238	17.093	1.00	16.41
ATOM	588	CD2	LEU	73	18.199	25.437	17.077	1.00	14.97
ATOM	589	C	LEU	73	17.804	29.708	18 102	1.00	7.12
ATOM	590	O	LEU	73	17.930	30 074	16.935	1.00	7 82
ATOM	591	N	ALA	74	17.541	30 607	19 036	1.00	6 72
ATOM	592	CA	ALA	74	17 201	31.967	18 766	1.00	6.46
ATOM	593	CB	ALA	74	16 742	32.662	20 042	1.00	7.96
ATOM	594	C	ALA	74	18 258	32.818	18.098	1.00	7.50
ATOM	595	O	ALA	74	19 423	32 697	18 490	1.00	8.38
ATOM	596	N	ILE	75	17.864	33 689	17.172	1.00	6.76
ATOM	597	CA	ILE	75	18 795	34.680	16.652	1.00	6.71
ATOM	598	CB	ILE	75	18 224	35.376	15.420	1.00	6.88
ATOM	599	CG2	ILE	75	18.044	34.424	14.239	1.00	8.21
ATOM	600	CG1	ILE	75	16.936	36.140	15 755	1.00	7.17
ATOM	601	CD1	ILE	75	16.522	37.151	14.715	1.00	9.71
ATOM	602	C	ILE	75	19.201	35 704	17.734	1.00	7.09
ATOM	603	O	ILE	75	18.546	35.810	18 781	1.00	6.89
ATOM	604	N	ALA	76	20.280	36.421	17.461	1.00	8 25
ATOM	605	CA	ALA	76	20 876	37 407	18.360	1.00	9 65
ATOM	606	CB	ALA	76	22 084	38.067	17.666	1.00	16.12
ATOM	607	C	ALA	76	19.886	38.445	18.838	1.00	8.48
ATOM	608	O	ALA	76	19.962	38.940	19.953	1.00	9.39
ATOM	609	N	ALA	77	18.905	38.810	18.002	1.00	8.30
ATOM	610	CA	ALA	77	17.911	39 800	18.374	1.00	9.45
ATOM	611	CB	ALA	77	16.992	40.064	17.179	1.00	10.84
ATOM	612	C	ALA	77	17 100	39.352	19.582	1.00	8.44
ATOM	613	O	ALA	77	16 541	40 191	20.299	1.00	10.71
ATOM	614	N	TYR	78	16.967	38 049	19.816	1.00	7.56
ATOM	615	CA	TYR	78	16.222	37.513	20 938	1.00	8.24
ATOM	616	CB	TYR	78	15 223	36.420	20.451	1.00	7.69
ATOM	617	CG	TYR	78	14.158	37 043	19.575	1.00	7.53
ATOM	618	CD1	TYR	78	14.272	36.972	18.193	1.00	7.61
ATOM	619	CE1	TYR	78	13 370	37.508	17 335	1.00	7 49
ATOM	620	CD2	TYR	78	13 050	37 728	20.079	1.00	8 66
ATOM	621	CE2	TYR	78	12 150	38.290	19.216	1.00	9 02
ATOM	622	CZ	TYR	78	12.291	38.173	17.845	1.00	8.23
ATOM	623	OH	TYR	78	11.357	38.805	17 028	1.00	10.37
ATOM	624	C	TYR	78	17.115	36.920	22 016	1.00	7 16
ATOM	625	O	TYR	78	16.681	36.716	23.134	1.00	10.37
ATOM	626	N	ASN	79	18 346	36.542	21.694	1.00	8.52
ATOM	627	CA	ASN	79	19.232	35.854	22 624	1.00	7.53
ATOM	628	CB	ASN	79	19 164	34.338	22 379	1.00	7.59
ATOM	629	CG	ASN	79	20.000	33.518	23 343	1.00	7.82
ATOM	630	OD1	ASN	79	20.942	34.010	23.962	1.00	8.62
ATOM	631	ND2	ASN	79	19.686	32.222	23 477	1.00	9.18
ATOM	632	C	ASN	79	20.653	36.401	22.394	1.00	8.94
ATOM	633	O	ASN	79	21.341	36.042	21.442	1.00	10.00
ATOM	634	N	LYS	80	21.086	37.226	23.348	1.00	9.67
ATOM	635	CA	LYS	80	22.403	37.853	23.279	1.00	11.21
ATOM	636	CB	LYS	80	22.575	38.808	24.473	1.00	14.70
ATOM	637	CG	LYS	80	21.697	40.035	24.385	1.00	20.93
ATOM	638	CD	LYS	80	21.970	41.007	25.532	1.00	25.64
ATOM	639	CE	LYS	80	21.540	42.420	25.219	1.00	29.22
ATOM	640	NZ	LYS	80	20.209	42.711	25.795	1.00	39.86
ATOM	641	C	LYS	80	23.565	36.877	23.274	1.00	10.80
ATOM	642	O	LYS	80	24.702	37.192	22.944	1.00	13.45
ATOM	643	N	GLU	81	23.349	35.630	23.706	1.00	10.06
ATOM	644	CA	GLU	81	24.436	34.666	23.722	1.00	11.25
ATOM	645	CB	GLU	81	24.060	33.385	24.505	1.00	11.80
ATOM	646	CG	GLU	81	23.668	33.565	25.948	1.00	15.18
ATOM	647	CD	GLU	81	23.394	32.322	26 768	1.00	16.40
ATOM	648	OE1	GLU	81	22.810	32.379	27.889	1.00	16.96
ATOM	649	OE2	GLU	81	23.688	31.185	26 315	1.00	21.03
ATOM	650	C	GLU	81	24.791	34.265	22 281	1.00	12.20
ATOM	651	O	GLU	81	25.838	33.655	22 069	1.00	14.12
ATOM	652	N	HIS	82	23.900	34.439	21 316	1.00	10.21
ATOM	653	CA	HIS	82	24 112	33.865	19.980	1.00	9.63

ATOM	654	CB	HIS	82	22.803	33.231	19.530	1.00	9.27
ATOM	655	CG	HIS	82	22.371	32.070	20.360	1.00	9.26
ATOM	656	CD2	HIS	82	23.068	31.323	21.257	1.00	10.67
ATOM	657	ND1	HIS	82	21.113	31.516	20.288	1.00	8.55
ATOM	658	CE1	HIS	82	21.063	30.500	21.141	1.00	8.43
ATOM	659	NE2	HIS	82	22.223	30.366	21 742	1.00	10.55
ATOM	660	C	HIS	82	24.567	34.933	19.029	1.00	10.23
ATOM	661	O	HIS	82	23.901	35.266	18 055	1.00	11.35
ATOM	662	N	GLN	83	25.726	35.507	19 295	1.00	12.56
ATOM	663	CA	GLN	83	26.203	36.634	18 507	1.00	13.52
ATOM	664	CB	GLN	83	27.470	37 164	19 181	1 00	16.22
ATOM	665	CG	GLN	83	27.163	37 925	20 478	1 00	19.23
ATOM	666	CD	GLN	83	26.294	39 148	20 300	1 00	20.38
ATOM	667	OE1	GLN	83	26.558	40 074	19 536	1 00	29.81
ATOM	668	NE2	GLN	83	25.191	39.208	21 046	1 00	22.46
ATOM	669	C	GLN	83	26 450	36 332	17 050	1 00	13 44
ATOM	670	O	GLN	83	26 392	37 262	16 246	1 00	15 10
ATOM	671	N	ASP	84	26 636	35 089	16 694	1.00	13.17
ATOM	**672**	**CA**	**ASP**	**84**	**26.862**	**34 722**	**15 292**	**1.00**	**14 01**
ATOM	673	CB	ASP	84	27.692	33 451	15 162	1.00	17.37
ATOM	674	CG	ASP	84	29 128	33 607	15 603	1 00	20 70
ATOM	675	OD1	ASP	84	29 618	34 762	15.567	1.00	24 40
ATOM	676	OD2	ASP	84	29 754	32.593	15.997	1.00	26 32
ATOM	677	C	ASP	84	25 622	34.566	14 450	1 00	12 94
ATOM	678	O	ASP	84	25 668	34.506	13 229	1 00	13 72
ATOM	679	N	GLN	85	24 472	34 466	15 125	1 00	12 76
ATOM	680	CA	GLN	85	23.186	34.270	14 473	1 00	11 48
ATOM	681	CB	GLN	85	22.324	33.390	15 381	1 00	11.21
ATOM	682	CG	GLN	85	22 791	31 971	15 552	1 00	11 91
ATOM	683	CD	GLN	85	21 795	31 109	16 278	1 00	10 83
ATOM	684	OE1	GLN	85	20.636	30.970	15 841	1 00	12 23
ATOM	685	NE2	GLN	85	22 225	30 557	17.380	1.00	9.17
ATOM	686	C	GLN	85	22 468	35.584	14.216	1.00	12.01
ATOM	687	O	GLN	85	21 590	36 041	14 977	1 00	14 96
ATOM	688	N	VAL	86	22 773	36.203	13 091	1 00	10 72
ATOM	689	CA	VAL	86	22 062	37 392	12.684	1.00	11 56
ATOM	690	CB	VAL	86	23.031	38.325	11 951	1 00	12 29
ATOM	691	CG1	VAL	86	22 341	39 541	11 368	1.00	16 28
ATOM	692	CG2	VAL	86	24 227	38 725	12 807	1 00	17 21
ATOM	693	C	VAL	86	20.862	36 994	11 853	1 00	11 74
ATOM	694	O	VAL	86	19 737	37 435	12 126	1 00	17 43
ATOM	695	N	ARG	87	21 060	36.084	10 898	1 00	8.55
ATOM	696	CA	ARG	87	20 044	35.624	9 972	1 00	7.72
ATOM	697	CB	ARG	87	20.635	35 441	8.552	1.00	8 11
ATOM	698	CG	ARG	87	21 203	36 706	7.959	1 00	8 47
ATOM	699	CD	ARG	87	21.842	36 462	6 599	1 00	7 75
ATOM	700	NE	ARG	87	20.829	36.173	5 609	1 00	7 39
ATOM	701	CZ	ARG	87	21.042	35.691	4.396	1 00	6.65
ATOM	702	NH1	ARG	87	22.260	35.389	3 959	1.00	8 68
ATOM	703	NH2	ARG	87	20 036	35.471	3 547	1.00	7 51
ATOM	704	C	ARG	87	19.410	34.289	10 332	1.00	7.27
ATOM	705	O	ARG	87	18 170	34 129	10.237	1 00	8.33
ATOM	706	N	ALA	88	20.206	33 270	10 609	1.00	7 40
ATOM	707	CA	ALA	88	19 749	31.876	10 750	1 00	6 92
ATOM	708	CB	ALA	88	20 760	30 869	10 254	1 00	8 59
ATOM	709	C	ALA	88	19.373	31 526	12 165	1.00	7.06
ATOM	710	O	ALA	88	20.138	31 793	13 084	1 00	9 57
ATOM	711	N	GLY	89	18 191	30 953	12 332	1.00	6 44
ATOM	712	CA	GLY	89	17.673	30.494	13 592	1 00	6 74
ATOM	713	C	GLY	89	16 222	30 872	13 801	1.00	6 22
ATOM	714	O	GLY	89	15 451	31.150	12.853	1 00	6.32
ATOM	715	N	TYR	90	15 811	30 854	15.062	1 00	6 31
ATOM	716	CA	TYR	90	14 439	31 063	15.460	1 00	6 72
ATOM	717	CB	TYR	90	14 009	30.142	16 623	1 00	7 29
ATOM	718	CG	TYR	90	12.552	29.793	16 487	1 00	6 81
ATOM	719	CD1	TYR	90	12 151	28 687	15 755	1 00	7 84
ATOM	720	CE1	TYR	90	10.830	28 357	15 592	1 00	8 96
ATOM	721	CD2	TYR	90	11 536	30 556	17 042	1 00	7 06
ATOM	722	CE2	TYR	90	10 193	30.257	16 837	1 00	8.48
ATOM	723	CZ	TYR	90	9.854	29.145	16 124	1 00	9.20
ATOM	724	OH	TYR	90	8.555	28.790	15 864	1 00	13.45
ATOM	725	C	TYR	90	14.191	32.541	15.802	1.00	6.30
ATOM	726	O	TYR	90	14.986	33.184	16.491	1.00	6.78

ATOM	727	N	TYR	91	13.035	33.030	15.320	1.00	6.07
ATOM	728	CA	TYR	91	12.554	34.384	15.484	1.00	6.47
ATOM	729	CB	TYR	91	12.252	35.025	14.135	1.00	6.78
ATOM	730	CG	TYR	91	13.392	35.277	13.209	1.00	6 23
ATOM	731	CD1	TYR	91	14.353	34.332	12.859	1.00	7 06
ATOM	732	CE1	TYR	91	15.364	34.597	11.962	1.00	7 29
ATOM	733	CD2	TYR	91	13.490	36 521	12.556	1.00	7.46
ATOM	734	CE2	TYR	91	14.486	36.776	11.634	1 00	7.96
ATOM	735	CZ	TYR	91	15.428	35 826	11 343	1.00	6.61
ATOM	736	OH	TYR	91	16.438	36.143	10 440	1.00	8 55
ATOM	737	C	TYR	91	11.289	34.262	16.334	1 00	5 71
ATOM	738	O	TYR	91	10.273	33.788	15 843	1 00	6 82
ATOM	739	N	LEU	92	11.385	34.629	17.619	1.00	6 69
ATOM	740	CA	LEU	92	10.306	34.337	18.569	1.00	6 33
ATOM	741	CB	LEU	92	10.873	34 371	19.987	1 00	7.20
ATOM	742	CG	LEU	92	11.700	33.188	20 466	1.00	7 89
ATOM	743	CD1	LEU	92	13.022	33 065	19.735	1.00	8.67
ATOM	744	CD2	LEU	92	11 888	33 261	21 985	1 00	10 35
ATOM	745	C	LEU	92	9.151	35.317	18.471	1.00	6.37
ATOM	746	O	LEU	92	9.284	36.491	18 161	1.00	7 36
ATOM	747	N	SER	93	7 976	34.786	18.810	1.00	7.12
ATOM	748	CA	SER	93	6 805	35 605	19.060	1.00	7 59
ATOM	749	CB	SER	93	5.523	34 794	19 013	1.00	8.96
ATOM	750	OG	SER	93	5.410	33 894	20 074	1 00	11.17
ATOM	751	C	SER	93	6.928	36 224	20.443	1.00	7.83
ATOM	752	O	SER	93	7 728	35.807	21.266	1.00	8 58
ATOM	753	N	ILE	94	6 100	37.213	20.688	1.00	9 38
ATOM	754	CA	ILE	94	6.029	37.865	22 016	1 00	9.91
ATOM	755	CB	ILE	94	6.640	39.280	21.992	1.00	10.58
ATOM	756	CG2	ILE	94	6.575	39.842	23 385	1.00	11.13
ATOM	757	CG1	ILE	94	8 051	39.304	21 385	1.00	11 02
ATOM	758	CD1	ILE	94	8 740	40 630	21.225	1.00	12.81
ATOM	759	C	ILE	94	4.550	37.947	22.376	1.00	9.85
ATOM	760	O	ILE	94	3.881	38.887	21 906	1.00	11.19
ATOM	761	N	PRO	95	4.006	36.948	23 046	1.00	10.93
ATOM	762	CD	PRO	95	4 693	35.749	23.520	1.00	12.42
ATOM	763	CA	PRO	95	2 560	36.878	23.342	1.00	12.23
ATOM	764	CB	PRO	95	2.394	35.670	24.234	1.00	13.83
ATOM	765	CG	PRO	95	3 555	34.807	23.867	1.00	13.55
ATOM	766	C	PRO	95	2 064	38.173	23 973	1.00	11.65
ATOM	767	O	PRO	95	2 791	38.800	24 780	1.00	12.20
ATOM	768	N	GLY	96	0.973	38.667	23.409	1.00	12.67
ATOM	769	CA	GLY	96	0.479	39.965	23.799	1.00	13.37
ATOM	770	C	GLY	96	0 933	41.142	22.976	1.00	12.23
ATOM	771	O	GLY	96	0 366	42.233	23 105	1.00	15.48
ATOM	772	N	LYS	97	1.992	40.975	22 189	1.00	12.23
ATOM	773	CA	LYS	97	2.637	42.048	21.444	1.00	11.30
ATOM	774	CB	LYS	97	3.947	42.410	22.187	1.00	12.24
ATOM	775	CG	LYS	97	3.784	42.828	23.625	1.00	13.52
ATOM	776	CD	LYS	97	3.087	44.147	23 758	1.00	15.77
ATOM	777	CE	LYS	97	3.019	44.549	25.226	1.00	18.45
ATOM	778	NZ	LYS	97	2.107	45.715	25.339	1.00	21.87
ATOM	779	C	LYS	97	2.977	41.783	19.977	1.00	10.88
ATOM	780	O	LYS	97	2.857	42.638	19.081	1.00	11.92
ATOM	781	N	LYS	98	3.453	40.583	19.691	1 00	10.38
ATOM	782	CA	LYS	98	3.913	40.149	18.374	1.00	9.59
ATOM	783	CB	LYS	98	5.442	40.215	18.332	1 00	12.06
ATOM	784	CG	LYS	98	6.093	39.618	17.105	1 00	11.30
ATOM	785	CD	LYS	98	7 604	39.879	17.116	1.00	10.99
ATOM	786	CE	LYS	98	8 338	39.370	15.908	1 00	10.76
ATOM	787	NZ	LYS	98	8 448	37.856	15.937	1.00	10.00
ATOM	788	C	LYS	98	3 462	38.723	18.145	1.00	9.52
ATOM	789	O	LYS	98	3 835	37.797	18.884	1.00	10.44
ATOM	790	N	ALA	99	2.674	38.529	17.108	1.00	8.69
ATOM	791	CA	ALA	99	2 095	37.221	16.865	1.00	8 30
ATOM	792	CB	ALA	99	0.771	37.440	16.107	1.00	11.01
ATOM	793	C	ALA	99	2 993	36.289	16.048	1.00	7 09
ATOM	794	O	ALA	99	3.091	35.086	16.291	1.00	8.34
ATOM	795	N	VAL	100	3.614	36.851	14.990	1.00	7.33
ATOM	796	CA	VAL	100	4 390	36.044	14.085	1.00	7.31
ATOM	797	CB	VAL	100	4.804	36.909	12.882	1.00	8.26
ATOM	798	CG1	VAL	100	5.854	37.965	13.230	1.00	9.84
ATOM	799	CG2	VAL	100	5.294	36.092	11.703	1.00	9.08

ATOM	800	C	VAL	100	5.636	35.463	14.759	1.00	6.77
ATOM	801	O	VAL	100	6.274	36.069	15.614	1.00	6.24
ATOM	802	N	GLU	101	6.039	34.294	14.261	1.00	5.93
ATOM	803	CA	GLU	101	7.275	33.647	14.643	1.00	5.89
ATOM	804	CB	GLU	101	7.164	32.758	15.864	1.00	6.83
ATOM	805	CG	GLU	101	6.194	31.599	15.714	1.00	9.01
ATOM	806	CD	GLU	101	5.993	30.900	17.058	1.00	11.15
ATOM	807	OE1	GLU	101	4.957	31.171	17.727	1.00	11.35
ATOM	808	OE2	GLU	101	6.839	30.033	17.396	1.00	16.56
ATOM	809	C	GLU	101	7.748	32.835	13.441	1.00	6.12
ATOM	810	O	GLU	101	6.989	32.513	12.532	1.00	6.44
ATOM	811	N	SER	102	9.047	32.564	13.384	1.00	6.02
ATOM	812	CA	SER	102	9.605	31.897	12.196	1.00	6.00
ATOM	813	CB	SER	102	9.725	32.906	11.058	1.00	6.77
ATOM	814	OG	SER	102	10.632	33.935	11.388	1.00	7.64
ATOM	815	C	SER	102	10.934	31.253	12.468	1.00	6.15
ATOM	816	O	SER	102	11.592	31.497	13.474	1.00	6.62
ATOM	817	N	PHE	103	11.367	30.433	11.517	1.00	5.73
ATOM	818	CA	PHE	103	12.670	29.792	11.506	1.00	5.88
ATOM	819	CB	PHE	103	12.521	28.294	11.756	1.00	6.37
ATOM	820	CG	PHE	103	13.795	27.476	11.663	1.00	6.21
ATOM	821	CD1	PHE	103	14.723	27.499	12.686	1.00	7.53
ATOM	822	CD2	PHE	103	14.024	26.650	10.562	1.00	7.03
ATOM	823	CE1	PHE	103	15.866	26.713	12.620	1.00	7.78
ATOM	824	CE2	PHE	103	15.167	25.887	10.483	1.00	6.93
ATOM	825	CZ	PHE	103	16.077	25.924	11.508	1.00	7.07
ATOM	826	C	PHE	103	13.319	30.018	10.149	1.00	5.84
ATOM	827	O	PHE	103	12.720	29.679	9.124	1.00	5.89
ATOM	828	N	CYS	104	14.505	30.596	10.128	1.00	5.38
ATOM	829	CA	CYS	104	15.244	30.888	8.907	1.00	5.34
ATOM	830	CB	CYS	104	15.669	32.368	8.935	1.00	6.38
ATOM	831	SG	CYS	104	16.693	32.902	7.544	1.00	7.14
ATOM	832	C	CYS	104	16.475	29.988	8.802	1.00	5.05
ATOM	833	O	CYS	104	17.202	29.802	9.794	1.00	5.55
ATOM	834	N	TYR	105	16.758	29.512	7.615	1.00	5.01
ATOM	835	CA	TYR	105	17.979	28.794	7.344	1.00	4.98
ATOM	836	CB	TYR	105	17.839	27.285	7.499	1.00	5.67
ATOM	837	CG	TYR	105	16.822	26.594	6.589	1.00	5.07
ATOM	838	CD1	TYR	105	17.258	25.856	5.491	1.00	5.34
ATOM	839	CE1	TYR	105	16.371	25.171	4.659	1.00	5.87
ATOM	840	CD2	TYR	105	15.469	26.551	6.883	1.00	5.19
ATOM	841	CE2	TYR	105	14.595	25.862	6.059	1.00	5.89
ATOM	842	CZ	TYR	105	15.045	25.169	4.966	1.00	5.38
ATOM	843	OH	TYR	105	14.141	24.495	4.169	1.00	6.39
ATOM	844	C	TYR	105	18.515	29.202	5.972	1.00	4.38
ATOM	845	O	TYR	105	17.778	29.622	5.072	1.00	5.26
ATOM	846	N	LEU	106	19.816	29.039	5.852	1.00	5.00
ATOM	847	CA	LEU	106	20.634	29.415	4.731	1.00	4.93
ATOM	848	CB	LEU	106	21.803	30.266	5.227	1.00	6.26
ATOM	849	CG	LEU	106	21.444	31.467	6.125	1.00	6.45
ATOM	850	CD1	LEU	106	22.709	32.219	6.477	1.00	8.37
ATOM	851	CD2	LEU	106	20.392	32.329	5.466	1.00	6.90
ATOM	852	C	LEU	106	21.121	28.188	3.948	1.00	4.77
ATOM	853	O	LEU	106	20.754	27.046	4.237	1.00	5.93
ATOM	854	N	ASN	107	21.991	28.473	2.983	1.00	4.96
ATOM	855	CA	ASN	107	22.654	27.437	2.187	1.00	5.23
ATOM	856	CB	ASN	107	23.803	28.147	1.434	1.00	5.83
ATOM	857	CG	ASN	107	24.424	27.280	0.353	1.00	5.32
ATOM	858	OD1	ASN	107	24.420	26.044	0.396	1.00	5.91
ATOM	859	ND2	ASN	107	24.989	27.988	-0.626	1.00	6.49
ATOM	860	C	ASN	107	23.225	26.347	3.079	1.00	4.82
ATOM	861	O	ASN	107	24.097	26.593	3.937	1.00	5.62
ATOM	862	N	PRO	108	22.771	25.095	2.881	1.00	4.96
ATOM	863	CD	PRO	108	21.595	24.677	2.118	1.00	5.43
ATOM	864	CA	PRO	108	23.345	23.973	3.639	1.00	5.82
ATOM	865	CB	PRO	108	22.516	22.773	3.134	1.00	6.84
ATOM	866	CG	PRO	108	21.194	23.377	2.749	1.00	6.32
ATOM	867	C	PRO	108	24.846	23.763	3.444	1.00	5.93
ATOM	868	O	PRO	108	25.533	23.129	4.274	1.00	6.51
ATOM	869	N	ASN	109	25.397	24.277	2.353	1.00	5.53
ATOM	870	CA	ASN	109	26.823	24.180	2.080	1.00	5.84
ATOM	871	CB	ASN	109	27.130	24.369	0.598	1.00	6.10
ATOM	872	CG	ASN	109	26.633	23.186	-0.200	1.00	5.51

ATOM	873	OD1	ASN	109	26 690	22.020	0.209	1.00	7.43
ATOM	874	ND2	ASN	109	26.165	23 491	-1 405	1 00	7.14
ATOM	875	C	ASN	109	27 652	25 150	2 920	1.00	5.95
ATOM	876	O	ASN	109	28 863	25.063	2.911	1.00	6.60
ATOM	877	N	PHE	110	27 032	26.060	3 672	1 00	6.52
ATOM	878	CA	PHE	110	27 727	26 943	4 602	1 00	6.64
ATOM	879	CB	PHE	110	26 984	28.235	4.934	1.00	6.86
ATOM	880	CG	PHE	110	26.793	29 203	3 781	1.00	6.62
ATOM	881	CD1	PHE	110	27.454	29.100	2.593	1.00	6.42
ATOM	882	CD2	PHE	110	25.889	30.238	3.919	1.00	7.13
ATOM	883	CE1	PHE	110	27.269	30.020	1 570	1 00	7.97
ATOM	884	CE2	PHE	110	25.698	31 178	2.917	1.00	7.73
ATOM	885	CZ	PHE	110	26 380	31 064	1 723	1 00	7.68
ATOM	886	C	PHE	110	28.010	26 131	5 870	1 00	6.42
ATOM	887	O	PHE	110	27.334	26 222	6.890	1.00	9.08
ATOM	888	N	THR	111	29.047	25 319	5 795	1.00	7.20
ATOM	889	CA	THR	111	29.543	24.473	6.858	1.00	7.97
ATOM	890	CB	THR	111	29.986	23.114	6.240	1.00	9.61
ATOM	891	OG1	THR	111	30.863	23.407	5.150	1.00	12.08
ATOM	892	CG2	THR	111	28.831	22.332	5.660	1 00	11.21
ATOM	893	C	THR	111	30.719	25 173	7 535	1 00	8.55
ATOM	894	O	THR	111	31.262	26 161	7 039	1.00	8.43
ATOM	895	N	PRO	112	31.158	24.669	8.690	1.00	10.82
ATOM	896	CD	PRO	112	30.500	23.646	9.514	1.00	12.34
ATOM	897	CA	PRO	112	32.284	25.317	9.365	1.00	10.76
ATOM	898	CB	PRO	112	32.454	24.403	10.591	1.00	12.53
ATOM	899	CG	PRO	112	31.035	23.971	10.884	1 00	13.67
ATOM	900	C	PRO	112	33.560	25.453	8 553	1.00	10.13
ATOM	901	O	PRO	112	34.293	26.449	8 719	1.00	12.02
ATOM	902	N	ASP	113	33.764	24 577	7 586	1.00	10.28
ATOM	903	CA	ASP	113	34.960	24 594	6.754	1.00	11.85
ATOM	904	CB	ASP	113	35.418	23.179	6.354	1.00	14.15
ATOM	905	CG	ASP	113	34.450	22.335	5.556	1.00	16.88
ATOM	906	OD1	ASP	113	34.697	21.122	5 265	1 00	17.94
ATOM	907	OD2	ASP	113	33.431	22.903	5 120	1 00	18.33
ATOM	908	C	ASP	113	34.779	25 485	5 516	1.00	10.04
ATOM	909	O	ASP	113	35.695	25 568	4 674	1.00	11.29
ATOM	910	N	HIS	114	33.614	26.058	5.256	1.00	8.19
ATOM	911	CA	HIS	114	33.388	26.853	4.066	1.00	7.72
ATOM	912	CB	HIS	114	31.924	27.234	3 945	1 00	8.19
ATOM	913	CG	HIS	114	31.514	27.896	2.661	1.00	7.35
ATOM	914	CD2	HIS	114	30.786	27.365	1.634	1.00	7.63
ATOM	915	ND1	HIS	114	31.853	29 194	2.350	1.00	7.74
ATOM	916	CE1	HIS	114	31.374	29.423	1.125	1.00	8.63
ATOM	917	NE2	HIS	114	30.698	28 385	0.701	1 00	8.22
ATOM	918	C	HIS	114	34.263	28.078	4.069	1 00	7.89
ATOM	919	O	HIS	114	34.363	28 705	5.126	1.00	8.23
ATOM	920	N	PRO	115	34.877	28.447	2.947	1.00	8.07
ATOM	921	CD	PRO	115	34.805	27.853	1.595	1.00	9 44
ATOM	922	CA	PRO	115	35.791	29 586	2.989	1 00	7 97
ATOM	923	CB	PRO	115	36.432	29.638	1.603	1.00	10.29
ATOM	924	CG	PRO	115	36.058	28.363	0.935	1.00	16 51
ATOM	925	C	PRO	115	35.213	30.906	3.451	1 00	8.16
ATOM	926	O	PRO	115	35.957	31.749	4.033	1 00	8.89
ATOM	927	N	ARG	116	33.935	31.156	3.245	1.00	7.57
ATOM	928	CA	ARG	116	33.282	32.366	3.687	1 00	8.05
ATOM	929	CB	ARG	116	32.055	32.649	2.831	1 00	9.75
ATOM	930	CG	ARG	116	32.363	33.041	1.398	1.00	11.43
ATOM	931	CD	ARG	116	33.024	34.444	1.316	1 00	17.12
ATOM	932	NE	ARG	116	32.909	34.976	-0.046	1.00	18.64
ATOM	933	CZ	ARG	116	33.267	36.202	-0.332	1 00	16.55
ATOM	934	NH1	ARG	116	33.732	37.005	0.626	1 00	18.90
ATOM	935	NH2	ARG	116	33.158	36.628	-1.550	1.00	19.38
ATOM	936	C	ARG	116	32.955	32.353	5.168	1 00	8.18
ATOM	937	O	ARG	116	32.905	33.426	5.807	1 00	10.55
ATOM	938	N	ILE	117	32.701	31.161	5.702	1 00	7.91
ATOM	939	CA	ILE	117	32.507	30.993	7.134	1.00	8.74
ATOM	940	CB	ILE	117	31.884	29.617	7.425	1 00	8.27
ATOM	941	CG2	ILE	117	31.909	29.337	8.920	1.00	10.79
ATOM	942	CG1	ILE	117	30.482	29.510	6.798	1 00	7.78
ATOM	943	CD1	ILE	117	29.478	30.458	7.376	1 00	9.72
ATOM	944	C	ILE	117	33.863	31.170	7.818	1 00	9.52
ATOM	945	O	ILE	117	33.956	31.893	8.820	1.00	10.02

ATOM	946	N	GLN	118	34.936	30.601	7.248	1.00	9.60
ATOM	947	CA	GLN	118	36.264	30.823	7.814	1.00	9.55
ATOM	948	CB	GLN	118	37.287	29.975	7.066	1.00	11.20
ATOM	949	CG	GLN	118	37.163	28.475	7.285	1.00	11.87
ATOM	950	CD	GLN	118	37.706	28.064	8.628	1.00	15.84
ATOM	951	OE1	GLN	118	38.799	28.509	9.021	1.00	16.95
ATOM	952	NE2	GLN	118	36.968	27.189	9.314	1.00	18.58
ATOM	953	C	GLN	118	36.624	32.301	7.782	1.00	10.34
ATOM	954	O	GLN	118	37.209	32.780	8.779	1.00	12.18
ATOM	955	N	ALA	119	36.307	33.008	6.719	1.00	10.58
ATOM	956	CA	ALA	119	36.652	34.437	6.577	1.00	11.17
ATOM	957	CB	ALA	119	36.675	34.884	5.141	1.00	11.90
ATOM	958	C	ALA	119	35.766	35.340	7.417	1.00	11.81
ATOM	959	O	ALA	119	35.975	36.547	7.593	1.00	13.51
ATOM	960	N	LYS	120	34.677	34.792	7.926	1.00	11.51
ATOM	961	CA	LYS	120	33.697	35.524	8.728	1.00	11.83
ATOM	962	CB	LYS	120	34.314	36.156	9.981	1.00	16.43
ATOM	963	CG	LYS	120	35.156	35.192	10.773	1.00	20.21
ATOM	964	CD	LYS	120	34.452	34.007	11.336	1.00	25.82
ATOM	965	CE	LYS	120	35.422	33.080	12.083	1.00	26.48
ATOM	966	NZ	LYS	120	36.364	32.304	11.194	1.00	23.67
ATOM	967	C	LYS	120	33.033	36.623	7.910	1.00	12.07
ATOM	968	O	LYS	120	32.701	37.698	8.413	1.00	13.32
ATOM	969	N	THR	121	32.773	36.290	6.647	1.00	11.59
ATOM	970	CA	THR	121	32.162	37.294	5.783	1.00	11.41
ATOM	971	CB	THR	121	32.158	36.758	4.336	1.00	11.74
ATOM	972	OG1	THR	121	33.515	36.460	3.947	1.00	14.18
ATOM	973	CG2	THR	121	31.617	37.825	3.394	1.00	13.26
ATOM	974	C	THR	121	30.742	37.599	6.199	1.00	10.30
ATOM	975	O	THR	121	30.016	36.627	6.442	1.00	9.38
ATOM	976	N	PRO	122	30.343	38.869	6.255	1.00	11.24
ATOM	977	CD	PRO	122	31.175	40.087	6.162	1.00	13.40
ATOM	978	CA	PRO	122	28.938	39.176	6.605	1.00	10.67
ATOM	979	CB	PRO	122	28.883	40.676	6.374	1.00	13.30
ATOM	980	CG	PRO	122	30.251	41.155	6.684	1.00	14.04
ATOM	981	C	PRO	122	27.932	38.454	5.721	1.00	8.90
ATOM	982	O	PRO	122	28.224	38.174	4.567	1.00	9.02
ATOM	983	N	THR	123	26.810	38.105	6.329	1.00	9.47
ATOM	984	CA	THR	123	25.660	37.447	5.729	1.00	8.42
ATOM	985	CB	THR	123	25.112	38.105	4.455	1.00	9.93
ATOM	986	OG1	THR	123	25.929	37.810	3.314	1.00	10.18
ATOM	987	CG2	THR	123	25.024	39.629	4.512	1.00	13.04
ATOM	988	C	THR	123	25.807	35.938	5.560	1.00	8.70
ATOM	989	O	THR	123	24.825	35.273	5.198	1.00	9.15
ATOM	990	N	HIS	124	26.994	35.395	5.833	1.00	8.34
ATOM	991	CA	HIS	124	27.189	33.957	5.798	1.00	7.64
ATOM	992	CB	HIS	124	28.524	33.584	5.149	1.00	7.45
ATOM	993	CG	HIS	124	28.726	34.113	3.780	1.00	7.00
ATOM	994	CD2	HIS	124	28.755	33.507	2.577	1.00	7.26
ATOM	995	ND1	HIS	124	28.998	35.449	3.557	1.00	7.88
ATOM	996	CE1	HIS	124	29.202	35.607	2.261	1.00	8.29
ATOM	997	NE2	HIS	124	29.032	34.478	1.632	1.00	7.93
ATOM	998	C	HIS	124	27.170	33.387	7.206	1.00	8.19
ATOM	999	O	HIS	124	27.888	33.913	8.056	1.00	9.17
ATOM	1000	N	GLU	125	26.413	32.313	7.455	1.00	7.36
ATOM	1001	CA	GLU	125	26.337	31.694	8.776	1.00	7.74
ATOM	1002	CB	GLU	125	25.166	32.230	9.604	1.00	8.77
ATOM	1003	CG	GLU	125	25.164	33.714	9.832	1.00	9.78
ATOM	1004	CD	GLU	125	23.885	34.235	10.445	1.00	9.41
ATOM	1005	OE1	GLU	125	23.057	33.439	10.972	1.00	12.02
ATOM	1006	OE2	GLU	125	23.791	35.476	10.373	1.00	12.25
ATOM	1007	C	GLU	125	26.118	30.196	8.567	1.00	7.57
ATOM	1008	O	GLU	125	25.581	29.787	7.521	1.00	8.65
ATOM	1009	N	VAL	126	26.505	29.398	9.557	1.00	7.88
ATOM	1010	CA	VAL	126	26.219	27.969	9.636	1.00	7.38
ATOM	1011	CB	VAL	126	27.281	27.246	10.488	1.00	8.22
ATOM	1012	CG1	VAL	126	26.979	25.754	10.561	1.00	9.54
ATOM	1013	CG2	VAL	126	28.686	27.497	9.941	1.00	9.36
ATOM	1014	C	VAL	126	24.843	27.785	10.272	1.00	7.39
ATOM	1015	O	VAL	126	24.564	28.311	11.344	1.00	8.29
ATOM	1016	N	ASN	127	23.951	27.081	9.554	1.00	6.96
ATOM	1017	CA	ASN	127	22.618	26.839	10.081	1.00	6.87
ATOM	1018	CB	ASN	127	21.832	25.948	9.120	1.00	6.56

ATOM	1019	CG	ASN	127	21 515	26 650	7.803	1.00	6.11
ATOM	1020	OD1	ASN	127	21.362	27 877	7.793	1 00	7.19
ATOM	1021	ND2	ASN	127	21 360	25.859	6.758	1 00	7.23
ATOM	1022	C	ASN	127	22 624	26.173	11.447	1 00	7.20
ATOM	1023	O	ASN	127	23.503	25.353	11.763	1.00	8.68
ATOM	1024	N	VAL	128	21 596	26 511	12 239	1.00	7.13
ATOM	1025	CA	VAL	128	21.284	25.849	13.501	1 00	7 06
ATOM	1026	CB	VAL	128	21.172	26 848	14.657	1.00	8 77
ATOM	1027	CG1	VAL	128	22.508	27 567	14 825	1 00	10 68
ATOM	1028	CG2	VAL	128	19.986	27.774	14.501	1 00	9 46
ATOM	1029	C	VAL	128	20.032	25.032	13 329	1.00	6 59
ATOM	1030	O	VAL	128	19.101	25.426	12.617	1.00	8.06
ATOM	1031	N	TRP	129	19.977	23.861	13.963	1.00	7 79
ATOM	1032	CA	TRP	129	18 884	22.914	13 812	1.00	7 98
ATOM	1033	CB	TRP	129	19.316	21.709	12 955	1.00	7 99
ATOM	1034	CG	TRP	129	19.671	22 145	11.553	1.00	7.47
ATOM	1035	CD2	TRP	129	18 743	22 448	10.496	1 00	6.77
ATOM	1036	CE2	TRP	129	19.486	22.838	9.368	1 00	6.74
ATOM	1037	CE3	TRP	129	17.353	22.428	10.400	1.00	6.42
ATOM	1038	CD1	TRP	129	20.887	22.349	11.033	1 00	8 81
ATOM	1039	NE1	TRP	129	20 809	22.765	9 721	1.00	8 43
ATOM	1040	CZ2	TRP	129	18 902	23.196	8.160	1.00	6 63
ATOM	1041	CZ3	TRP	129	16.754	22.796	9.207	1.00	7 42
ATOM	1042	CH2	TRP	129	17.553	23.187	8.120	1.00	6 84
ATOM	1043	C	TRP	129	18.434	22.394	15.187	1 00	8.10
ATOM	1044	O	TRP	129	19.266	22.268	16.108	1 00	9.20
ATOM	1045	N	PRO	130	17.158	22.038	15.321	1.00	9.10
ATOM	1046	CD	PRO	130	16.078	22.208	14.338	1.00	11.04
ATOM	1047	CA	PRO	130	16.684	21.410	16 563	1 00	10 04
ATOM	1048	CB	PRO	130	15 190	21 366	16.377	1.00	12 74
ATOM	1049	CG	PRO	130	14.987	21.348	14.930	1.00	12 90
ATOM	1050	C	PRO	130	17 295	20.019	16.674	1.00	10.76
ATOM	1051	O	PRO	130	17 902	19.473	15.742	1.00	10.41
ATOM	1052	N	ASP	131	17.139	19.412	17.840	1.00	12.19
ATOM	1053	CA	ASP	131	17.611	18.063	18.062	1.00	13 83
ATOM	1054	CB	ASP	131	17.311	17.695	19.499	1.00	20.75
ATOM	1055	CG	ASP	131	18 290	18.307	20.474	1.00	30.05
ATOM	1056	OD1	ASP	131	19.218	19 075	20.122	1.00	41 54
ATOM	1057	OD2	ASP	131	18.111	17.974	21.678	1.00	44 79
ATOM	1058	C	ASP	131	16.864	17.077	17.175	1.00	12.28
ATOM	1059	O	ASP	131	15.643	17.091	17.104	1.00	11 37
ATOM	1060	N	GLU	132	17.632	16 204	16.561	1.00	12.37
ATOM	1061	CA	GLU	132	17.032	15 236	15.660	1.00	12.37
ATOM	1062	CB	GLU	132	18 140	14.416	14.986	1.00	14 40
ATOM	1063	CG	GLU	132	17.667	13.221	14.169	1.00	14.02
ATOM	1064	CD	GLU	132	17 004	13.617	12.890	1.00	14 20
ATOM	1065	OE1	GLU	132	17 327	14 733	12.391	1 00	13.96
ATOM	1066	OE2	GLU	132	16.222	12.787	12.395	1.00	14 71
ATOM	1067	C	GLU	132	16 028	14.309	16.327	1.00	13.05
ATOM	1068	O	GLU	132	15.022	13 953	15.730	1 00	13 21
ATOM	1069	N	THR	133	16.283	13.922	17.576	1 00	15 02
ATOM	1070	CA	THR	133	15.337	13 065	18 267	1.00	17 13
ATOM	1071	CB	THR	133	15.911	12.663	19.645	1.00	19.10
ATOM	1072	OG1	THR	133	16.214	13 817	20 436	1 00	30.56
ATOM	1073	CG2	THR	133	17.200	11 914	19 407	1 00	21.80
ATOM	1074	C	THR	133	14.003	13.738	18 504	1.00	14.81
ATOM	1075	O	THR	133	12.976	13 052	18.539	1.00	18.31
ATOM	1076	N	LYS	134	13.992	15.065	18.681	1.00	14.08
ATOM	1077	CA	LYS	134	12.738	15 763	18.943	1.00	14.05
ATOM	1078	CB	LYS	134	13.028	17 072	19.683	1.00	16.10
ATOM	1079	CG	LYS	134	13.566	16.783	21.105	1.00	21.50
ATOM	1080	CD	LYS	134	13.739	18 052	21.912	1.00	24.72
ATOM	1081	CE	LYS	134	13.962	17.851	23.411	1.00	29.07
ATOM	1082	NZ	LYS	134	15.380	17.498	23.673	1.00	35.66
ATOM	1083	C	LYS	134	11.982	16.084	17.673	1.00	11.72
ATOM	1084	O	LYS	134	10.764	16.268	17.697	1.00	12.75
ATOM	1085	N	HIS	135	12.768	16.210	16.602	1.00	10.34
ATOM	1086	CA	HIS	135	12.229	16.559	15.278	1.00	9.70
ATOM	1087	CB	HIS	135	12.568	18.014	14.927	1.00	10.46
ATOM	1088	CG	HIS	135	11.859	18.971	15.855	1.00	11.60
ATOM	1089	CD2	HIS	135	10.625	19.519	15.664	1.00	11.74
ATOM	1090	ND1	HIS	135	12.334	19.405	17.077	1.00	13.42
ATOM	1091	CE1	HIS	135	11.390	20.219	17.592	1.00	10.37

ATOM	1092	NE2	HIS	135	10.358	20.261	16.753	1.00	14.68
ATOM	1093	C	HIS	135	12.753	15.614	14.207	1.00	9.49
ATOM	1094	O	HIS	135	13.491	16.005	13.302	1.00	8.95
ATOM	1095	N	PRO	136	12.410	14.336	14.298	1.00	10.29
ATOM	1096	CD	PRO	136	11.539	13.714	15.288	1.00	12.71
ATOM	1097	CA	PRO	136	12.996	13.348	13.367	1.00	10.63
ATOM	1098	CB	PRO	136	12.331	12.025	13.738	1.00	13.20
ATOM	1099	CG	PRO	136	11.373	12.308	14.822	1.00	15.42
ATOM	1100	C	PRO	136	12 727	13.656	11.902	1.00	9.37
ATOM	1101	O	PRO	136	11 583	13.947	11.540	1.00	10.11
ATOM	1102	N	GLY	137	13 801	13.643	11.131	1.00	9.15
ATOM	1103	CA	GLY	137	13 642	13.906	9.700	1 00	8.92
ATOM	1104	C	GLY	137	13.568	15.351	9.281	1 00	8.41
ATOM	1105	O	GLY	137	13 604	15.660	8.076	1.00	8.62
ATOM	1106	N	PHE	138	13 438	16.290	10.230	1 00	7.77
ATOM	1107	CA	PHE	138	13 189	17.683	9.858	1 00	7.53
ATOM	1108	CB	PHE	138	12 791	18.533	11.069	1 00	9.20
ATOM	1109	CG	PHE	138	12.676	20.014	10.773	1 00	8.61
ATOM	1110	CD1	PHE	138	11.623	20.502	9.999	1.00	8.98
ATOM	1111	CD2	PHE	138	13 628	20.897	11.264	1.00	8.98
ATOM	1112	CE1	PHE	138	11.598	21 878	9.728	1.00	9.24
ATOM	1113	CE2	PHE	138	13 584	22.238	11.007	1.00	9 39
ATOM	1114	CZ	PHE	138	12.555	22.730	10.231	1.00	8 60
ATOM	1115	C	PHE	138	14 355	18.318	9.123	1.00	6.57
ATOM	1116	O	PHE	138	14.355	18.953	8.090	1.00	6 31
ATOM	1117	N	GLN	139	15 553	18.234	9.700	1.00	7 35
ATOM	1118	CA	GLN	139	16.718	18.827	9.045	1.00	7.49
ATOM	1119	CB	GLN	139	17.990	18.600	9.867	1.00	7.76
ATOM	1120	CG	GLN	139	19.211	19 123	9.164	1.00	8.03
ATOM	1121	CD	GLN	139	20.475	19.034	10.008	1.00	9.61
ATOM	1122	OE1	GLN	139	20.452	18 629	11.194	1.00	11.81
ATOM	1123	NE2	GLN	139	21.556	19 403	9.361	1.00	10.42
ATOM	1124	C	GLN	139	16.898	18.263	7.634	1.00	6 36
ATOM	1125	O	GLN	139	17.148	19 042	6 703	1.00	6.70
ATOM	1126	N	ASP	140	16.792	16.962	7.476	1.00	7 41
ATOM	1127	CA	ASP	140	16.966	16.359	6.153	1.00	8.02
ATOM	1128	CB	ASP	140	17.014	14.845	6 267	1.00	10 06
ATOM	1129	CG	ASP	140	18.185	14.414	7.143	1.00	12.56
ATOM	1130	OD1	ASP	140	19.263	15.008	7.017	1.00	15.40
ATOM	1131	OD2	ASP	140	18.010	13.419	7.863	1.00	17.99
ATOM	1132	C	ASP	140	15.903	16.836	5.173	1.00	7.03
ATOM	1133	O	ASP	140	16.195	17.225	4.012	1.00	7.37
ATOM	1134	N	PHE	141	14.649	16.886	5.632	1.00	6.76
ATOM	1135	CA	PHE	141	13.592	17.404	4.806	1.00	6.92
ATOM	1136	CB	PHE	141	12.241	17.315	5 525	1.00	8.28
ATOM	1137	CG	PHE	141	11.180	18.059	4 700	1.00	10.59
ATOM	1138	CD1	PHE	141	10.649	17.398	3 585	1.00	12.85
ATOM	1139	CD2	PHE	141	10.766	19.326	4.979	1.00	12 09
ATOM	1140	CE1	PHE	141	9.773	18.045	2.730	1.00	14.79
ATOM	1141	CE2	PHE	141	9.946	20.027	4.097	1.00	12 80
ATOM	1142	CZ	PHE	141	9.514	19.385	2.960	1.00	15 56
ATOM	1143	C	PHE	141	13.898	18.843	4.381	1.00	6.10
ATOM	1144	O	PHE	141	13 715	19 227	3.224	1.00	5.52
ATOM	1145	N	ALA	142	14 235	19.692	5.355	1.00	5.91
ATOM	1146	CA	ALA	142	14 436	21.113	5.109	1 00	6.07
ATOM	1147	CB	ALA	142	14.597	21.835	6.444	1.00	6.15
ATOM	1148	C	ALA	142	15.593	21.396	4.153	1.00	5.38
ATOM	1149	O	ALA	142	15.534	22.273	3.289	1.00	5.69
ATOM	1150	N	GLU	143	16.660	20.630	4.306	1.00	5.79
ATOM	1151	CA	GLU	143	17.811	20.759	3.404	1.00	5.89
ATOM	1152	CB	GLU	143	19.021	19.977	3.912	1.00	6.66
ATOM	1153	CG	GLU	143	19.647	20.589	5.171	1.00	6.49
ATOM	1154	CD	GLU	143	20.818	19 857	5.742	1.00	8.57
ATOM	1155	OE1	GLU	143	20.986	18.661	5.468	1.00	15.50
ATOM	1156	OE2	GLU	143	21.529	20.401	6.607	1.00	8.03
ATOM	1157	C	GLU	143	17.426	20.335	1.982	1.00	6 15
ATOM	1158	O	GLU	143	17.798	21.030	1.046	1.00	6 03
ATOM	1159	N	GLN	144	16.717	19.195	1.852	1.00	6.24
ATOM	1160	CA	GLN	144	16.249	18.793	0.519	1.00	5.81
ATOM	1161	CB	GLN	144	15.582	17.418	0.622	1.00	7.33
ATOM	1162	CG	GLN	144	15.034	16.900	-0.718	1.00	9.38
ATOM	1163	CD	GLN	144	16.102	16.723	-1.755	1.00	11.31
ATOM	1164	OE1	GLN	144	16.165	17.336	-2.852	1.00	15.13

ATOM	1165	NE2	GLN	144	17 017	15.794	-1.443	1.00	13.37
ATOM	1166	C	GLN	144	15.322	19.843	-0.068	1.00	6.08
ATOM	1167	O	GLN	144	15 367	20.113	-1.286	1.00	6.65
ATOM	1168	N	TYR	145	14.450	20.464	0.723	1.00	5.44
ATOM	1169	CA	TYR	145	13.552	21.492	0.249	1.00	5.36
ATOM	1170	CB	TYR	145	12.562	21 956	1 318	1.00	5.45
ATOM	1171	CG	TYR	145	11 718	23.094	0 785	1.00	5.34
ATOM	1172	CD1	TYR	145	10.850	22.844	-0.266	1.00	5.77
ATOM	1173	CE1	TYR	145	10.113	23.856	-0.832	1.00	5.40
ATOM	1174	CD2	TYR	145	11.863	24.392	1 209	1.00	6.05
ATOM	1175	CE2	TYR	145	11.128	25.428	0.632	1.00	5.52
ATOM	1176	CZ	TYR	145	10.260	25 146	-0.376	1 00	4 90
ATOM	1177	OH	TYR	145	9.505	26 126	-1.002	1 00	6.57
ATOM	1178	C	TYR	145	14.350	22.668	-0.324	1.00	4.85
ATOM	1179	O	TYR	145	14.009	23.173	-1 384	1.00	5.67
ATOM	1180	N	TYR	146	15.400	23.055	0.370	1.00	5 22
ATOM	1181	CA	TYR	146	16.294	24 134	-0.108	1 00	5.07
ATOM	1182	CB	TYR	146	17.492	24.302	0.818	1 00	6.31
ATOM	1183	CG	TYR	146	18.356	25.533	0.554	1.00	5.63
ATOM	1184	CD1	TYR	146	18.217	26.654	1.367	1 00	4.93
ATOM	1185	CE1	TYR	146	18.975	27.804	1.191	1 00	4.66
ATOM	1186	CD2	TYR	146	19.292	25.595	-0.471	1.00	5.91
ATOM	1187	CE2	TYR	146	20.050	26.728	-0.673	1.00	5.60
ATOM	1188	CZ	TYR	146	19.892	27.816	0.151	1.00	5.33
ATOM	1189	OH	TYR	146	20.681	28.929	-0 076	1 00	6.01
ATOM	1190	C	TYR	146	16.740	23.831	-1.547	1 00	4.88
ATOM	1191	O	TYR	146	16.630	24.691	-2 413	1.00	5.89
ATOM	1192	N	TRP	147	17.186	22.580	-1 792	1.00	5.20
ATOM	1193	CA	TRP	147	17.650	22.244	-3.129	1 00	5.95
ATOM	1194	CB	TRP	147	18.544	20.995	-3.105	1 00	6.61
ATOM	1195	CG	TRP	147	19.730	21.259	-2 221	1.00	6.71
ATOM	1196	CD2	TRP	147	20.675	22.345	-2 390	1.00	6.87
ATOM	1197	CE2	TRP	147	21.598	22.227	-1.334	1.00	7.71
ATOM	1198	CE3	TRP	147	20.828	23.398	-3.303	1.00	7.63
ATOM	1199	CD1	TRP	147	20.127	20.576	-1.120	1.00	7.42
ATOM	1200	NE1	TRP	147	21.230	21.118	-0.574	1.00	7.49
ATOM	1201	CZ2	TRP	147	22.641	23.133	-1.198	1.00	8.32
ATOM	1202	CZ3	TRP	147	21.873	24.299	-3.147	1.00	8.76
ATOM	1203	CH2	TRP	147	22.774	24.162	2.079	1.00	8.40
ATOM	1204	C	TRP	147	16.514	22.124	-4.123	1.00	5.56
ATOM	1205	O	TRP	147	16.697	22.484	-5.295	1.00	6.90
ATOM	1206	N	ASP	148	15.333	21.663	-3.736	1.00	5.62
ATOM	1207	CA	ASP	148	14.192	21.610	-4.644	1.00	6.73
ATOM	1208	CB	ASP	148	13.006	20.892	-3.990	1.00	7.41
ATOM	1209	CG	ASP	148	13.180	19.397	-3.794	1.00	9.94
ATOM	1210	OD1	ASP	148	14.107	18.824	-4.385	1.00	11.03
ATOM	1211	OD2	ASP	148	12.308	18.805	-3.115	1.00	12.94
ATOM	1212	C	ASP	148	13.807	23.013	-5.076	1.00	6.41
ATOM	1213	O	ASP	148	13.602	23.288	-6.281	1.00	6.39
ATOM	1214	N	VAL	149	13.678	23.959	-4.112	1.00	5.67
ATOM	1215	CA	VAL	149	13.287	25.330	-4.472	1.00	5.45
ATOM	1216	CB	VAL	149	12.664	26.047	-3.279	1.00	5.40
ATOM	1217	CG1	VAL	149	13.656	26.460	-2.202	1.00	5.95
ATOM	1218	CG2	VAL	149	11.883	27.265	-3.771	1.00	6.77
ATOM	1219	C	VAL	149	14.421	26.084	-5.158	1.00	5.36
ATOM	1220	O	VAL	149	14.173	26.951	-6.016	1.00	5.85
ATOM	1221	N	PHE	150	15.669	25.750	-4.879	1.00	5.71
ATOM	1222	CA	PHE	150	16.795	26.267	-5.635	1.00	5.05
ATOM	1223	CB	PHE	150	18.111	25.675	-5.056	1.00	6.21
ATOM	1224	CG	PHE	150	19 374	26.154	-5.764	1.00	6.04
ATOM	1225	CD1	PHE	150	20.158	27.164	-5.267	1.00	7.32
ATOM	1226	CD2	PHE	150	19 840	25.565	-6 911	1.00	7.41
ATOM	1227	CE1	PHE	150	21 279	27.602	-5 932	1.00	7.77
ATOM	1228	CE2	PHE	150	20.926	26.005	-7 649	1.00	8.49
ATOM	1229	CZ	PHE	150	21 686	27.017	-7.119	1.00	7 48
ATOM	1230	C	PHE	150	16.626	25.887	-7 102	1.00	5 89
ATOM	1231	O	PHE	150	16.841	26.726	-8.004	1.00	6 52
ATOM	1232	N	GLY	151	16.276	24.637	-7.351	1.00	6.70
ATOM	1233	CA	GLY	151	16.124	24.168	-8.744	1.00	6.74
ATOM	1234	C	GLY	151	15.012	24.887	-9.476	1.00	6.45
ATOM	1235	O	GLY	151	15.150	25 293	-10.619	1.00	7.27
ATOM	1236	N	LEU	152	13.867	25 094	-8.825	1.00	6.82
ATOM	1237	CA	LEU	152	12.787	25.878	-9.404	1.00	6.24

ATOM	1238	CB	LEU	152	11.582	25.881	-8.452	1.00	6.29
ATOM	1239	CG	LEU	152	10.452	26.859	-8.828	1.00	7.25
ATOM	1240	CD1	LEU	152	9.864	26.532	-10.214	1.00	9.19
ATOM	1241	CD2	LEU	152	9.358	26.832	-7.763	1.00	7.05
ATOM	1242	C	LEU	152	13.269	27.298	-9.669	1.00	6.42
ATOM	1243	O	LEU	152	13.025	27.864	-10.743	1.00	7.31
ATOM	1244	N	SER	153	13.998	27.874	-8.702	1.00	5.98
ATOM	1245	CA	SER	153	14 442	29.262	-8.845	1.00	6.16
ATOM	1246	CB	SER	153	15 068	29.742	-7 541	1.00	6 44
ATOM	1247	OG	SER	153	14 090	29 755	-6 522	1.00	6 18
ATOM	1248	C	SER	153	15 424	29 413	-10 000	1.00	6 14
ATOM	1249	O	SER	153	15 368	30 420	-10 740	1.00	6 53
ATOM	1250	N	SER	154	16.284	28 436	-10.217	1.00	6 45
ATOM	1251	CA	SER	154	17 220	28.495	-11.340	1.00	7 39
ATOM	1252	CB	SER	154	18 126	27.271	-11.278	1.00	8.84
ATOM	1253	OG	SER	154	18 981	27.292	10.189	1.00	13.14
ATOM	1254	C	SER	154	16 418	28 472	-12.643	1.00	7 57
ATOM	1255	O	SER	154	16.742	29.253	-13 563	1.00	8 31
ATOM	1256	N	ALA	155	15.408	27.630	-12.737	1.00	6.91
ATOM	1257	CA	ALA	155	14.550	27 622	-13.938	1.00	7.39
ATOM	1258	CB	ALA	155	13 530	26 520	-13.807	1 00	7.77
ATOM	1259	C	ALA	155	13 878	28 964	-14 140	1 00	6.87
ATOM	1260	O	ALA	155	13.895	29 538	-15 242	1.00	7 86
ATOM	1261	N	LEU	156	13.323	29 547	-13 083	1.00	6 99
ATOM	1262	CA	LEU	156	12 656	30 860	-13.176	1 00	5 86
ATOM	1263	CB	LEU	156	12 035	31 279	-12.838	1 00	5 92
ATOM	1264	CG	LEU	156	10 864	30 434	-11.365	1 00	5 99
ATOM	1265	CD1	LEU	156	10.480	30 809	-9 936	1 00	8 87
ATOM	1266	CD2	LEU	156	9 686	30.596	-12 284	1.00	11.48
ATOM	1267	C	LEU	156	13 640	31.933	-13.642	1 00	6 11
ATOM	1268	O	LEU	156	13 287	32.805	-14.447	1.00	7.28
ATOM	1269	N	LEU	157	14 884	32 880	-13 141	1 00	6.74
ATOM	1270	CA	LEU	157	15.898	32.863	-13.543	1 00	7.25
ATOM	1271	CB	LEU	157	17.152	32.739	-12.694	1.00	6.79
ATOM	1272	CG	LEU	157	17 073	33.236	-11.250	1.00	7.78
ATOM	1273	CD1	LEU	157	18.408	33.026	-10.580	1.00	8.46
ATOM	1274	CD2	LEU	157	16.631	34.672	-11.145	1 00	9 12
ATOM	1275	C	LEU	157	16 227	32.748	-15.028	1.00	6 91
ATOM	1276	O	LEU	157	16 580	33.763	-15.638	1.00	7.24
ATOM	1277	N	LYS	158	16.142	31.561	-15.606	1 00	7 38
ATOM	1278	CA	LYS	158	16.335	31.410	-17.057	1 00	7 07
ATOM	1279	CB	LYS	158	16.381	29.927	-17 407	1 00	9 01
ATOM	1280	CG	LYS	158	17 574	29.170	-16.887	1.00	10 48
ATOM	1281	CD	LYS	158	17.541	27.683	-17.122	1 00	13 42
ATOM	1282	CE	LYS	158	18 743	27.039	-16.407	1 00	18 16
ATOM	1283	NZ	LYS	158	18.743	25.572	-16.586	1 00	18.72
ATOM	1284	C	LYS	158	15 185	32.121	-17 782	1 00	7 00
ATOM	1285	O	LYS	158	15 447	32.806	-18 770	1 00	9 09
ATOM	1286	N	GLY	159	13.951	32 032	-17.281	1 00	7.17
ATOM	1287	CA	GLY	159	12.834	32.752	-17 873	1 00	7.22
ATOM	1288	C	GLY	159	13.038	34.252	-17.763	1.00	6.90
ATOM	1289	O	GLY	159	12.756	34.973	-18.731	1 00	7.59
ATOM	1290	N	TYR	160	13 443	34 771	-16.620	1.00	7.51
ATOM	1291	CA	TYR	160	13.674	36 230	-16.489	1.00	6.84
ATOM	1292	CB	TYR	160	14 004	36.595	-15 059	1.00	7.03
ATOM	1293	CG	TYR	160	12 831	36.759	-14 120	1.00	6.77
ATOM	1294	CD1	TYR	160	12 421	35.752	-13 251	1.00	6.69
ATOM	1295	CE1	TYR	160	11 353	35.915	-12 430	1.00	7.61
ATOM	1296	CD2	TYR	160	12 097	37.948	-14 093	1.00	7.26
ATOM	1297	CE2	TYR	160	11 013	38.108	-13 247	1.00	7.77
ATOM	1298	CZ	TYR	160	10 643	37.083	-12 380	1.00	7.26
ATOM	1299	OH	TYR	160	9 594	37.202	-11 495	1.00	8.86
ATOM	1300	C	TYR	160	14 756	36.704	-17 446	1.00	6.38
ATOM	1301	O	TYR	160	14 653	37.777	-18 003	1.00	7.25
ATOM	1302	N	ALA	161	15 849	35.968	-17 537	1.00	7.30
ATOM	1303	CA	ALA	161	16 929	36 375	-18 438	1.00	7.63
ATOM	1304	CB	ALA	161	18 083	35 387	-18 293	1.00	9.13
ATOM	1305	C	ALA	161	16 414	36 456	-19 886	1.00	7.60
ATOM	1306	O	ALA	161	16 688	37 458	-20 577	1.00	8.23
ATOM	1307	N	LEU	162	15 755	35 401	-20 331	1.00	7.75
ATOM	1308	CA	LEU	162	15 234	35 423	-21 721	1.00	7.67
ATOM	1309	CB	LEU	162	14 537	34.094	-22 022	1.00	7.94
ATOM	1310	CG	LEU	162	15.447	32.872	-22.168	1.00	8.36

ATOM	1311	CD1	LEU	162	14 644	31.593	-22 325	1.00	10.23
ATOM	1312	CD2	LEU	162	16.390	33 093	-23.326	1 00	10.26
ATOM	1313	C	LEU	162	14 256	36.582	-21 871	1.00	7.87
ATOM	1314	O	LEU	162	14 228	37 234	-22.926	1 00	8 10
ATOM	1315	N	ALA	163	13 396	36.840	-20 874	1 00	7 67
ATOM	1316	CA	ALA	163	12 422	37 934	-20.922	1 00	8 06
ATOM	1317	CB	ALA	163	11.568	37.986	-19 658	1 00	8 57
ATOM	1318	C	ALA	163	13 122	39 278	-21.162	1 00	8.14
ATOM	1319	O	ALA	163	12.527	40 158	-21.830	1 00	9 20
ATOM	1320	N	LEU	164	14 320	39.445	-20.607	1.00	8 56
ATOM	1321	CA	LEU	164	15 075	40 688	-20.710	1.00	8 69
ATOM	1322	CB	LEU	164	15 881	40.917	-19.409	1.00	9 34
ATOM	1323	CG	LEU	164	15.007	41 231	-18.199	1.00	9.92
ATOM	1324	CD1	LEU	164	15.707	40.869	-16.893	1.00	11.23
ATOM	1325	CD2	LEU	164	14.532	42 665	-18.193	1 00	11.47
ATOM	1326	C	LEU	164	15.968	40.800	-21.920	1.00	8.43
ATOM	1327	O	LEU	164	16.728	41 751	-22.068	1.00	10.53
ATOM	1328	N	GLY	165	15.876	39.849	-22 823	1.00	9.22
ATOM	1329	CA	GLY	165	16 653	39.841	-24 034	1 00	9.48
ATOM	1330	C	GLY	165	18.044	39.299	-23.843	1.00	9.27
ATOM	1331	O	GLY	165	18.900	39 539	-24.692	1.00	10.21
ATOM	1332	N	LYS	166	18.298	38 579	-22.754	1.00	9 48
ATOM	1333	CA	LYS	166	19 627	38.033	-22.452	1 00	9 96
ATOM	1334	CB	LYS	166	19 982	38.274	-20.984	1.00	9 69
ATOM	1335	CG	LYS	166	19 946	39.708	-20 549	1 00	11 03
ATOM	1336	CD	LYS	166	20.825	40 606	-21.352	1 00	14.43
ATOM	1337	CE	LYS	166	20.799	42 029	-20.820	1 00	18 44
ATOM	1338	NZ	LYS	166	21.480	42.980	-21.738	1.00	27.60
ATOM	1339	C	LYS	166	19.669	36.535	-22.725	1.00	9 64
ATOM	1340	O	LYS	166	18.611	35.926	-22.985	1.00	11.70
ATOM	1341	N	GLU	167	20.837	35.917	-22.660	1.00	9.56
ATOM	1342	CA	GLU	167	20.979	34.447	-22.758	1.00	10.09
ATOM	1343	CB	GLU	167	22.436	34.051	-22.993	1.00	12 65
ATOM	1344	CG	GLU	167	23.380	34.300	-21.838	1 00	22 48
ATOM	1345	CD	GLU	167	23.665	33.149	-20.891	1.00	25.40
ATOM	1346	OE1	GLU	167	23.311	31.984	-21.190	1.00	32.34
ATOM	1347	OE2	GLU	167	24.326	33.330	-19.840	1.00	31.11
ATOM	1348	C	GLU	167	20.484	33.838	-21.438	1.00	9.49
ATOM	1349	O	GLU	167	20.519	34.524	-20.407	1 00	10.35
ATOM	1350	N	GLU	168	19.999	32.587	-21.453	1.00	9.82
ATOM	1351	CA	GLU	168	19.298	32.071	-20.295	1 00	9.33
ATOM	1352	CB	GLU	168	18.638	30.725	-20.586	1.00	10.98
ATOM	1353	CG	GLU	168	19.586	29.555	-20.607	1.00	11 58
ATOM	1354	CD	GLU	168	18.897	28.248	-20.881	1.00	12.24
ATOM	1355	OE1	GLU	168	19.518	27.191	-20.621	1.00	16.73
ATOM	1356	OE2	GLU	168	17.710	28.209	-21.238	1.00	15 75
ATOM	1357	C	GLU	168	20.121	31.991	-19.021	1.00	9 76
ATOM	1358	O	GLU	168	19.500	31.919	-17.957	1.00	10 27
ATOM	1359	N	ASN	169	21 440	31.959	-19.098	1.00	11 16
ATOM	1360	CA	ASN	169	22.256	31.849	-17.894	1.00	11 83
ATOM	1361	CB	ASN	169	23 467	30.962	-18.200	1.00	17.37
ATOM	1362	CG	ASN	169	23 037	29.534	-18.442	1.00	25.58
ATOM	1363	OD1	ASN	169	23.422	28.858	-19.416	1.00	36 44
ATOM	1364	ND2	ASN	169	22 234	29.059	-17.485	1.00	33.88
ATOM	1365	C	ASN	169	22 665	33.191	-17.342	1.00	10.67
ATOM	1366	O	ASN	169	23.471	33 254	-16.423	1.00	10.87
ATOM	1367	N	PHE	170	22.101	34 292	-17.818	1.00	9.81
ATOM	1368	CA	PHE	170	22.503	35.641	-17.397	1.00	9.43
ATOM	1369	CB	PHE	170	21.676	36 690	-18.110	1.00	10.54
ATOM	1370	CG	PHE	170	21.970	38 143	-17 807	1.00	10.68
ATOM	1371	CD1	PHE	170	22.971	38.748	-18 561	1.00	11.73
ATOM	1372	CD2	PHE	170	21.249	38 844	-16.841	1.00	11.45
ATOM	1373	CE1	PHE	170	23.277	40 069	-18 325	1.00	13.22
ATOM	1374	CE2	PHE	170	21.601	40 156	-16 603	1.00	13.30
ATOM	1375	CZ	PHE	170	22.581	40 787	-17.369	1.00	13.73
ATOM	1376	C	PHE	170	22.466	35 905	-15 896	1.00	9.39
ATOM	1377	O	PHE	170	23.388	36 499	-15 313	1.00	10.53
ATOM	1378	N	PHE	171	21.414	35 405	-15.249	1.00	9.21
ATOM	1379	CA	PHE	171	21.328	35 485	-13 799	1.00	9.20
ATOM	1380	CB	PHE	171	19.882	35 735	-13.353	1.00	9.39
ATOM	1381	CG	PHE	171	19.270	37.023	-13.840	1.00	9.53
ATOM	1382	CD1	PHE	171	18.199	36 958	-14.716	1.00	8.43
ATOM	1383	CD2	PHE	171	19.751	38.247	-13.409	1.00	9.70

ATOM	1384	CE1	PHE	171	17.637	38.140	-15.183	1.00	9.69
ATOM	1385	CE2	PHE	171	19.208	39.427	-13.881	1.00	11.03
ATOM	1386	CZ	PHE	171	18.138	39.369	-14 774	1 00	9.32
ATOM	1387	C	PHE	171	21.798	34.187	-13 158	1 00	9.45
ATOM	1388	O	PHE	171	22.557	34 196	-12 160	1 00	10.11
ATOM	1389	N	ALA	172	21.386	33 058	-13 727	1 00	8 64
ATOM	1390	CA	ALA	172	21.662	31 758	-13 141	1 00	9 25
ATOM	1391	CB	ALA	172	20.995	30 619	-13 907	1 00	11 46
ATOM	1392	C	ALA	172	23.144	31 456	-12.935	1 00	9 80
ATOM	1393	O	ALA	172	23.515	30.728	-12.017	1 00	9 88
ATOM	1394	N	ARG	173	24.014	32 048	-13 757	1 00	10 46
ATOM	1395	CA	ARG	173	25.456	31.811	-13 607	1 00	10.74
ATOM	1396	CB	ARG	173	26.229	32.377	-14 804	1 00	12.02
ATOM	1397	CG	ARG	173	26.252	33.888	-14 845	1 00	14 37
ATOM	1398	CD	ARG	173	26.528	34 507	-16.235	1.00	22 60
ATOM	1399	NE	ARG	173	26 118	35 904	-16 110	1.00	29 23
ATOM	1400	CZ	ARG	173	26 204	37 054	-16.666	1.00	27 71
ATOM	1401	NH1	ARG	173	26.785	37 249	-17.871	1.00	38 25
ATOM	**1402**	**NH2**	**ARG**	**173**	**25.671**	**38.128**	**-16.092**	**1.00**	**20.56**
ATOM	1403	C	ARG	173	25 967	32 398	-12 321	1.00	10.00
ATOM	1404	O	ARG	173	27 059	31.984	-11 891	1 00	12 18
ATOM	1405	N	HIS	174	25.265	33 305	-11.671	1 00	8 86
ATOM	1406	CA	HIS	174	25 621	33 884	-10.385	1.00	8 97
ATOM	1407	CB	HIS	174	25 281	35 380	-10.393	1.00	9 34
ATOM	1408	CG	HIS	174	25 986	36 119	-11 478	1.00	11 02
ATOM	1409	CD2	HIS	174	27 272	36.548	-11 356	1 00	13.05
ATOM	1410	ND1	HIS	174	25.560	36 543	-12.686	1 00	15.18
ATOM	1411	CE1	HIS	174	26.537	37 180	-13.306	1 00	16.14
ATOM	1412	NE2	HIS	174	27.575	37 238	-12.505	1 00	17 60
ATOM	1413	C	HIS	174	24 864	33.267	-9 203	1 00	8 17
ATOM	1414	O	HIS	174	25 053	33.704	-8.067	1 00	10 44
ATOM	1415	N	PHE	175	24.093	32.251	-9.482	1.00	8.57
ATOM	1416	CA	PHE	175	23.230	31.536	-8.516	1.00	7.07
ATOM	1417	CB	PHE	175	21.772	31.678	-8.967	1.00	7.09
ATOM	1418	CG	PHE	175	20.743	31.096	-8.020	1 00	6 00
ATOM	1419	CD1	PHE	175	19.888	30 101	-8.409	1.00	6 11
ATOM	1420	CD2	PHE	175	20.644	31.566	-6.725	1 00	6 48
ATOM	1421	CE1	PHE	175	18.940	29 615	-7.548	1 00	7.35
ATOM	1422	CE2	PHE	175	19.709	31.073	-5.837	1 00	7.65
ATOM	1423	CZ	PHE	175	18 834	30.096	-6.266	1.00	7 87
ATOM	1424	C	PHE	175	23.686	30 089	-8 421	1.00	7 96
ATOM	1425	O	PHE	175	23.298	29.250	-9.248	1.00	8.40
ATOM	1426	N	LYS	176	24 602	29 813	-7 494	1.00	7.81
ATOM	1427	CA	LYS	176	25 320	28 576	-7 473	1.00	7 94
ATOM	1428	CB	LYS	176	26.813	28.901	-7 674	1.00	10 84
ATOM	1429	CG	LYS	176	27 215	29 556	-8.956	1.00	15 51
ATOM	1430	CD	LYS	176	28 584	30 190	-8.877	1.00	23.52
ATOM	1431	CE	LYS	176	28.905	31 261	-7.886	1.00	31.75
ATOM	1432	NZ	LYS	176	28.155	32.528	-7.591	1.00	30 18
ATOM	1433	C	LYS	176	25.206	27.890	-6.114	1.00	7.44
ATOM	1434	O	LYS	176	25.237	28.596	-5.079	1.00	7.02
ATOM	1435	N	PRO	177	25.115	26.568	-6 114	1.00	7 06
ATOM	1436	CD	PRO	177	25 016	25.639	-7 241	1 00	8 87
ATOM	1437	CA	PRO	177	24 978	25 874	-4.842	1 00	7 22
ATOM	1438	CB	PRO	177	24 960	24 392	-5.244	1 00	9 12
ATOM	1439	CG	PRO	177	24.494	24 351	-6 632	1 00	12 20
ATOM	1440	C	PRO	177	26 107	26.128	-3 866	1 00	6.45
ATOM	1441	O	PRO	177	25 842	26 133	-2.655	1.00	6.96
ATOM	1442	N	ASP	178	27.355	26 340	-4.296	1 00	7.00
ATOM	1443	CA	ASP	178	28 432	26 494	-3 322	1 00	7.82
ATOM	1444	CB	ASP	178	29 784	26.223	-3.996	1 00	7.64
ATOM	1445	CG	ASP	178	30 055	24 770	-4 225	1 00	8.62
ATOM	1446	OD1	ASP	178	29 305	23.888	-3 752	1 00	10.49
ATOM	1447	OD2	ASP	178	31 072	24.504	-4.927	1 00	9 66
ATOM	1448	C	ASP	178	28 418	27.826	-2.624	1 00	8 41
ATOM	1449	O	ASP	178	29 053	27.922	-1.567	1 00	11.48
ATOM	1450	N	ASP	179	27 747	28.844	-3.172	1.00	7.61
ATOM	1451	CA	ASP	179	27 868	30.160	-2.558	1.00	8.48
ATOM	1452	CB	ASP	179	29 017	31.003	-3.110	1.00	14.39
ATOM	1453	CG	ASP	179	28.896	31.215	-4.582	1.00	17.08
ATOM	1454	OD1	ASP	179	27 769	31.231	-5.087	1.00	18.23
ATOM	1455	OD2	ASP	179	29.974	31.247	-5.214	1.00	29.01
ATOM	1456	C	ASP	179	26.622	30.999	-2.437	1.00	6.67

ATOM	1457	O	ASP	179	26.723	32 118	-1.937	1.00	7.91
ATOM	1458	N	THR	180	25.459	30.574	-2.903	1.00	6.15
ATOM	1459	CA	THR	180	24.291	31.397	-2.818	1.00	5.45
ATOM	1460	CB	THR	180	23.061	30 717	-3.495	1.00	6.14
ATOM	1461	OG1	THR	180	21.933	31 564	-3.275	1.00	6.60
ATOM	1462	CG2	THR	180	22.728	29 384	-2.872	1.00	7.19
ATOM	1463	C	THR	180	23.929	31 823	-1.404	1.00	5.42
ATOM	1464	O	THR	180	23.995	31 022	-0 488	1.00	6.17
ATOM	1465	N	LEU	181	23 568	33 098	-1 291	1.00	5 82
ATOM	1466	CA	LEU	181	23 100	33.709	-0.086	1.00	5.33
ATOM	1467	CB	LEU	181	23.535	35.173	0.000	1.00	5.68
ATOM	1468	CG	LEU	181	25 031	35.342	0 214	1.00	7.12
ATOM	1469	CD1	LEU	181	25.527	36 714	-0.116	1.00	9.05
ATOM	1470	CD2	LEU	181	25.431	34 952	1 631	1.00	9 04
ATOM	1471	C	LEU	181	21 596	33 554	0.126	1 00	5.36
ATOM	1472	O	LEU	181	21 002	34.159	1.018	1.00	5 78
ATOM	1473	N	ALA	182	20 943	32 746	-0 705	1 00	5.62
ATOM	1474	CA	ALA	182	19.499	32 518	-0.607	1.00	5.07
ATOM	1475	CB	ALA	182	19.041	31.560	-1 713	1.00	5 84
ATOM	1476	C	ALA	182	19.111	31 916	0 741	1.00	5.26
ATOM	1477	O	ALA	182	19 829	31.152	1.390	1.00	5.11
ATOM	1478	N	SER	183	17 929	32.266	1.215	1.00	5.45
ATOM	1479	CA	SER	183	17.387	31 766	2.475	1.00	5.43
ATOM	1480	CB	SER	183	17.361	32.908	3 478	1 00	6 48
ATOM	1481	OG	SER	183	16.484	33 920	3 050	1 00	7 39
ATOM	1482	C	SER	183	15 975	31.229	2.287	1.00	5.28
ATOM	1483	O	SER	183	15 220	31.691	1.430	1.00	5.14
ATOM	1484	N	VAL	184	15.624	30.298	3.167	1.00	4.72
ATOM	1485	CA	VAL	184	14 272	29 833	3.379	1.00	4.18
ATOM	1486	CB	VAL	184	14.156	28 311	3.410	1 00	4.82
ATOM	1487	CG1	VAL	184	12.784	27 827	3.825	1.00	5.78
ATOM	1488	CG2	VAL	184	14.574	27 702	2.084	1.00	5.85
ATOM	1489	C	VAL	184	13 803	30.392	4.728	1.00	4.63
ATOM	1490	O	VAL	184	14.563	30.341	5.712	1.00	5.58
ATOM	1491	N	VAL	185	12.571	30.872	4.785	1.00	5.40
ATOM	1492	CA	VAL	185	11.960	31 260	6.049	1 00	5.11
ATOM	1493	CB	VAL	185	11.732	32 758	6.222	1.00	5.44
ATOM	1494	CG1	VAL	185	11.355	33.084	7.659	1.00	7.04
ATOM	1495	CG2	VAL	185	12.974	33.556	5.824	1.00	7.05
ATOM	1496	C	VAL	185	10.664	30.482	6.215	1.00	5.37
ATOM	1497	O	VAL	185	9.793	30.537	5.354	1.00	6.79
ATOM	1498	N	LEU	186	10 525	29.766	7.340	1.00	5.04
ATOM	1499	CA	LEU	186	9 312	29.030	7.659	1 00	5.37
ATOM	1500	CB	LEU	186	9 608	27.651	8.191	1.00	6.74
ATOM	1501	CG	LEU	186	10.519	26 783	7.329	1 00	7.22
ATOM	1502	CD1	LEU	186	10 783	25 457	8.026	1 00	8.08
ATOM	1503	CD2	LEU	186	9 933	26.589	5.923	1.00	7.11
ATOM	1504	C	LEU	186	8.512	29.883	8.645	1.00	5.24
ATOM	1505	O	LEU	186	8.777	29.826	9.854	1.00	6.31
ATOM	1506	N	ILE	187	7.577	30 701	8.165	1 00	5.56
ATOM	1507	CA	ILE	187	6.864	31.641	9.010	1.00	5.65
ATOM	1508	CB	ILE	187	6.589	32 984	8.305	1.00	6.04
ATOM	1509	CG2	ILE	187	5.916	33 986	9.250	1 00	7.75
ATOM	1510	CG1	ILE	187	7.804	33.601	7.633	1.00	6.80
ATOM	1511	CD1	ILE	187	7.550	34.739	6.667	1.00	7.49
ATOM	1512	C	ILE	187	5.511	31.068	9 440	1.00	6.09
ATOM	1513	O	ILE	187	4.740	30.565	8.617	1.00	6.78
ATOM	1514	N	ARG	188	5.253	31.145	10 736	1.00	6.56
ATOM	1515	CA	ARG	188	3.970	30.800	11.332	1.00	6.28
ATOM	1516	CB	ARG	188	4.130	29.967	12.611	1.00	7.38
ATOM	1517	CG	ARG	188	2.799	29.623	13 245	1.00	7.70
ATOM	1518	CD	ARG	188	2.926	29.038	14.641	1.00	9.29
ATOM	1519	NE	ARG	188	1.588	28.821	15.185	1.00	11.11
ATOM	1520	CZ	ARG	188	1.357	28.454	16 431	1.00	12.61
ATOM	1521	NH1	ARG	188	2.357	28.232	17 264	1.00	16.10
ATOM	1522	NH2	ARG	188	0.090	28 327	16 815	1 00	16.40
ATOM	1523	C	ARG	188	3.224	32.081	11 714	1.00	6.29
ATOM	1524	O	ARG	188	3.714	32.892	12 499	1.00	7.23
ATOM	1525	N	TYR	189	2.053	32.239	11 099	1.00	6.43
ATOM	1526	CA	TYR	189	1.129	33.301	11 534	1.00	6.36
ATOM	1527	CB	TYR	189	0.565	33.997	10 302	1.00	7.87
ATOM	1528	CG	TYR	189	1.432	35.109	9 770	1.00	7.69
ATOM	1529	CD1	TYR	189	2.245	34.959	8 649	1.00	8.11

ATOM	1530	CE1	TYR	189	3.023	36.028	8.202	1.00	8.55
ATOM	1531	CD2	TYR	189	1.433	36.344	10.407	1.00	8.98
ATOM	1532	CE2	TYR	189	2.188	37.425	9.969	1.00	9.17
ATOM	1533	CZ	TYR	189	2.981	37.241	8.841	1.00	8.58
ATOM	1534	OH	TYR	189	3 728	38.328	8.379	1.00	11.03
ATOM	1535	C	TYR	189	0 033	32.562	12.300	1.00	7.25
ATOM	1536	O	TYR	189	-0 678	31.766	11.696	1.00	8 05
ATOM	1537	N	PRO	190	-0.137	32.811	13.576	1.00	6 97
ATOM	1538	CD	PRO	190	0 666	33.760	14.412	1.00	7 48
ATOM	1539	CA	PRO	190	-1 091	32.037	14.367	1.00	7.93
ATOM	1540	CB	PRO	190	-0 484	32 215	15.773	1.00	9 03
ATOM	1541	CG	PRO	190	-0 032	33 667	15 732	1.00	8 65
ATOM	1542	C	PRO	190	-2 516	32.564	14 390	1.00	7 31
ATOM	1543	O	PRO	190	-2 768	33.746	14 183	1.00	7 83
ATOM	1544	N	TYR	191	-3 428	31.672	14 740	1 00	8 07
ATOM	1545	CA	TYR	191	-4 758	32.035	15 189	1 00	8 05
ATOM	1546	CB	TYR	191	-5 741	30.882	15 033	1.00	9.47
ATOM	1547	CG	TYR	191	-7 089	31 164	15.645	1.00	8.74
ATOM	**1548**	**CD1**	**TYR**	**191**	**-7 981**	**32 032**	**15 052**	**1.00**	**10 94**
ATOM	1549	CE1	TYR	191	-9 203	32 283	15 640	1.00	12 35
ATOM	1550	CD2	TYR	191	-7 434	30 628	16.867	1.00	11 98
ATOM	1551	CE2	TYR	191	-8 662	30.860	17 464	1 00	13.36
ATOM	1552	CZ	TYR	191	-9.520	31.710	16.847	1.00	13 52
ATOM	1553	OH	TYR	191	-10 758	31 949	17 411	1 00	20 40
ATOM	1554	C	TYR	191	-4 634	32 252	16 687	1 00	8 41
ATOM	1555	O	TYR	191	-4 028	31 574	17 419	1 00	10 11
ATOM	1556	N	LEU	192	-5 188	33 493	17.089	1.00	9 02
ATOM	1557	CA	LEU	192	-5.170	33.901	18 490	1.00	9.80
ATOM	1558	CB	LEU	192	-4 106	35 000	18 751	1 00	10.70
ATOM	1559	CG	LEU	192	-2 670	34 624	18 449	1 00	11 38
ATOM	1560	CD1	LEU	192	-1 779	35.835	18.366	1.00	15 17
ATOM	1561	CD2	LEU	192	-2 195	33 545	19 376	1.00	14.95
ATOM	1562	C	LEU	192	-6 524	34 466	18.870	1 00	11 59
ATOM	1563	O	LEU	192	-7.087	35 298	18.167	1.00	13 64
ATOM	1564	N	ASP	193	-7 038	34 106	20.036	1 00	14 51
ATOM	1565	CA	ASP	193	-8 305	34 590	20 567	1 00	17.44
ATOM	1566	C	ASP	193	-8.162	34 839	22 054	1 00	18.14
ATOM	1567	O	ASP	193	-8 094	33 884	22.833	1 00	20 69
ATOM	1568	CB	ASP	193	-9 424	33.558	20.361	1.00	19 90
ATOM	1569	CG	ASP	193	-10 778	34 035	20.844	1 00	22.56
ATOM	1570	OD1	ASP	193	-10 950	35 239	21 071	1 00	31.28
ATOM	1571	OD2	ASP	193	-11 705	33 195	20 904	1 00	31 66
ATOM	1572	N	PRO	194	-8 007	36 055	22.502	1 00	19 75
ATOM	1573	CD	PRO	194	-7 751	36.353	23 938	1 00	21.02
ATOM	1574	CA	PRO	194	-8 074	37.262	21 705	1 00	20.34
ATOM	1575	CB	PRO	194	-8.358	38.337	22 780	1 00	22 22
ATOM	1576	CG	PRO	194	-7 623	37.846	23 976	1 00	23 24
ATOM	1577	C	PRO	194	-6 794	37.553	20 961	1.00	18 30
ATOM	1578	O	PRO	194	-5.732	37.174	21 441	1 00	20.47
ATOM	1579	N	TYR	195	-6.908	38.261	19 844	1 00	16 09
ATOM	1580	CA	TYR	195	-5 729	38.654	19.057	1.00	13 39
ATOM	1581	CB	TYR	195	-6.063	38.748	17.591	1.00	11 89
ATOM	1582	CG	TYR	195	-4 857	38 589	16.678	1.00	10.40
ATOM	1583	CD1	TYR	195	-4 733	37.428	15 902	1 00	9 05
ATOM	1584	CE1	TYR	195	-3 668	37.229	15 052	1 00	9.43
ATOM	1585	CD2	TYR	195	-3 867	39.556	16 532	1 00	11 25
ATOM	1586	CE2	TYR	195	-2.801	39.370	15 678	1.00	10.47
ATOM	1587	CZ	TYR	195	-2.706	38 217	14 940	1.00	9 27
ATOM	1588	OH	TYR	195	-1 631	38.037	14 084	1 00	10 15
ATOM	1589	C	TYR	195	-5 251	40.015	19 570	1.00	16 02
ATOM	1590	O	TYR	195	-6 045	40.984	19 547	1.00	19 50
ATOM	1591	N	PRO	196	-4 015	40.101	20 038	1 00	19 81
ATOM	1592	CD	PRO	196	-2 943	39 107	19 944	1 00	20 75
ATOM	1593	CA	PRO	196	-3 555	41.366	20 632	1.00	22.65
ATOM	1594	CB	PRO	196	-2.113	41 061	21 050	1.00	24 78
ATOM	1595	CG	PRO	196	-1 702	39.919	20 178	1.00	25 22
ATOM	1596	C	PRO	196	-3.528	42.534	19.659	1.00	21.80
ATOM	1597	O	PRO	196	-2 893	42.411	18.610	1.00	18.33
ATOM	1598	N	ALA	197	-4 121	43.655	20.069	1.00	20.80
ATOM	1599	CA	ALA	197	-4.137	44.850	19.209	1.00	17.10
ATOM	1600	CB	ALA	197	-4.992	45.932	19.849	1.00	22.74
ATOM	1601	C	ALA	197	-2.736	45.332	18.943	1.00	16.42
ATOM	1602	O	ALA	197	-2.416	45.845	17.884	1.00	14.48

ATOM	1603	N	ALA	198	-1 806	45.093	19.872	1.00	18.94
ATOM	1604	CA	ALA	198	-0 457	45.551	19.663	1.00	18 82
ATOM	1605	CB	ALA	198	0.389	45.537	20.917	1.00	21 76
ATOM	1606	C	ALA	198	0 247	44.830	18.532	1.00	20 09
ATOM	1607	O	ALA	198	1.209	45.380	17.989	1.00	20 87
ATOM	1608	N	ALA	199	-0 282	43.655	18.148	1.00	18.02
ATOM	1609	CA	ALA	199	0.284	42.883	17.055	1.00	20.04
ATOM	1610	CB	ALA	199	0.131	41.377	17.305	1.00	22.29
ATOM	1611	C	ALA	199	-0 405	43.201	15.745	1.00	17 65
ATOM	1612	O	ALA	199	-0 143	42.526	14.746	1.00	19 33
ATOM	1613	N	ILE	200	-1.272	44.187	15.758	1.00	14.55
ATOM	1614	CA	ILE	200	-2 007	44.619	14.572	1.00	12 89
ATOM	1615	CB	ILE	200	-3 524	44.490	14.735	1.00	12.11
ATOM	1616	CG2	ILE	200	-4 273	44 933	13.481	1.00	15.92
ATOM	1617	CG1	ILE	200	-3.933	43 079	15.169	1.00	12 87
ATOM	1618	CD1	ILE	200	-5.369	42.887	15.559	1.00	15 12
ATOM	1619	C	ILE	200	-1.604	46.049	14.242	1.00	12.80
ATOM	1620	O	ILE	200	-1 722	46.945	15.061	1.00	15.14
ATOM	1621	N	LYS	201	-1 079	46 217	13.030	1.00	12.46
ATOM	1622	CA	LYS	201	-0 723	47 561	12.585	1 00	13.42
ATOM	1623	C	LYS	201	-1 842	48.108	11 712	1.00	12 82
ATOM	1624	O	LYS	201	-2.682	47 341	11 198	1.00	12 98
ATOM	1625	CB	LYS	201	0.575	47 555	11.793	1 00	15 55
ATOM	1626	CG	LYS	201	1 786	47.469	12 720	1 00	22 73
ATOM	1627	CD	LYS	201	2 968	47 442	11 792	1.00	30.21
ATOM	1628	CE	LYS	201	3 330	45.969	11 633	1.00	33 55
ATOM	1629	NZ	LYS	201	4 352	45.602	12.674	1.00	44 14
ATOM	1630	N	THR	202	-1.844	49 414	11.525	1 00	12 30
ATOM	1631	CA	THR	202	-2.896	50 018	10 731	1 00	12 03
ATOM	1632	CB	THR	202	-3.769	50.900	11.654	1 00	14 94
ATOM	1633	OG1	THR	202	-4 283	50.136	12.749	1.00	20 93
ATOM	1634	CG2	THR	202	-4 968	51 401	10.876	1.00	16.31
ATOM	1635	C	THR	202	-2.353	50.883	9.608	1.00	10.86
ATOM	1636	O	THR	202	-1.574	51.831	9.881	1.00	12.79
ATOM	1637	N	ALA	203	-2.710	50.593	8.362	1.00	10.61
ATOM	1638	CA	ALA	203	-2 246	51.412	7.251	1 00	10.61
ATOM	1639	CB	ALA	203	-2.554	50.704	5.923	1.00	10.92
ATOM	1640	C	ALA	203	-2.907	52.771	7.177	1.00	11.45
ATOM	1641	O	ALA	203	-3 927	53.003	7.798	1 00	12.75
ATOM	1642	N	ALA	204	-2.316	53.701	6.418	1 00	13.11
ATOM	1643	CA	ALA	204	-2.922	55.016	6.262	1.00	14.24
ATOM	1644	CB	ALA	204	-2.081	55.921	5.383	1 00	17.62
ATOM	1645	C	ALA	204	-4.312	54.951	5.666	1.00	15.18
ATOM	1646	O	ALA	204	-5.116	55.828	5.979	1 00	18.40
ATOM	1647	N	ASP	205	-4.656	53.935	4.910	1.00	14.70
ATOM	1648	CA	ASP	205	-6.010	53.765	4.378	1.00	15.08
ATOM	1649	CB	ASP	205	-5.939	53.130	2 979	1.00	14.53
ATOM	1650	CG	ASP	205	-5.558	51.681	2.919	1.00	13.86
ATOM	1651	OD1	ASP	205	-5.431	51.036	3.978	1.00	13.58
ATOM	1652	OD2	ASP	205	-5.414	51.137	1 785	1.00	14.56
ATOM	1653	C	ASP	205	-6.958	53.042	5.330	1.00	13.99
ATOM	1654	O	ASP	205	-8.100	52.729	4 944	1.00	16.91
ATOM	1655	N	GLY	206	-6.470	52.672	6.523	1.00	13 46
ATOM	1656	CA	GLY	206	-7.305	51.999	7.498	1.00	13.34
ATOM	1657	C	GLY	206	-7.215	50.496	7.536	1.00	12 65
ATOM	1658	O	GLY	206	-7.688	49.850	8.492	1.00	15 08
ATOM	1659	N	THR	207	-6.523	49.909	6.562	1.00	11 08
ATOM	1660	CA	THR	207	-6.383	48.461	6.501	1.00	10 33
ATOM	1661	CB	THR	207	-5.728	48.047	5.186	1.00	10.43
ATOM	1662	OG1	THR	207	-6.475	48.593	4.068	1.00	11.13
ATOM	1663	CG2	THR	207	-5.730	46.528	5.000	1.00	11.62
ATOM	1664	C	THR	207	-5.542	47.948	7.669	1 00	10.83
ATOM	1665	O	THR	207	-4 460	48.451	7.944	1 00	11.23
ATOM	1666	N	LYS	208	-6 047	46.906	8.322	1 00	10.43
ATOM	1667	CA	LYS	208	-5 328	46.251	9.393	1.00	10.06
ATOM	1668	CB	LYS	208	-6 299	45.472	10.281	1 00	10.90
ATOM	1669	CG	LYS	208	-7.310	46.400	10.977	1.00	15.45
ATOM	1670	CD	LYS	208	-8.216	45.550	11.860	1.00	21.10
ATOM	1671	CE	LYS	208	-9.070	46.277	12.858	1.00	25.92
ATOM	1672	NZ	LYS	208	-10.228	45.455	13 309	1.00	35.34
ATOM	1673	C	LYS	208	-4.281	45.341	8.753	1.00	8.69
ATOM	1674	O	LYS	208	-4.631	44.523	7.893	1.00	8.73
ATOM	1675	N	LEU	209	-3.058	45.470	9.211	1.00	8.66

ATOM	1676	CA	LEU	209	-1.912	44.745	8.686	1.00	8.20
ATOM	1677	CB	LEU	209	-0.919	45.780	8.126	1.00	8.17
ATOM	1678	CG	LEU	209	-1.407	46.777	7.084	1.00	8.96
ATOM	1679	CD1	LEU	209	-0.263	47.711	6.737	1.00	10.26
ATOM	1680	CD2	LEU	209	-1.959	46.077	5.837	1.00	9.92
ATOM	1681	C	LEU	209	-1.149	43.969	9.733	1.00	8.39
ATOM	1682	O	LEU	209	-1.077	44.308	10.910	1.00	9.60
ATOM	1683	N	SER	210	-0.445	42.944	9.250	1.00	7.50
ATOM	1684	CA	SER	210	0.555	42.241	10.017	1.00	8.27
ATOM	1685	CB	SER	210	0.481	40.717	9.879	1.00	9.13
ATOM	1686	OG	SER	210	-0.677	40.154	10.458	1.00	10.38
ATOM	1687	C	SER	210	1.958	42.709	9.625	1.00	8.82
ATOM	1688	O	SER	210	2.867	42.559	10.430	1.00	11.07
ATOM	1689	N	PHE	211	2.153	43.228	8.404	1.00	8.41
ATOM	1690	CA	PHE	211	3.465	43.640	7.944	1.00	8.42
ATOM	1691	CB	PHE	211	4.294	42.502	7.351	1.00	9.04
ATOM	1692	CG	PHE	211	5.784	42.797	7.169	1.00	8.29
ATOM	1693	CD1	PHE	211	6.656	42.844	8.237	1.00	9.90
ATOM	**1694**	**CD2**	**PHE**	**211**	**6.316**	**43.023**	**5.916**	**1.00**	**8.43**
ATOM	1695	CE1	PHE	211	8.014	43.064	8.074	1.00	9.71
ATOM	1696	CE2	PHE	211	7.649	43.256	5.735	1.00	9.43
ATOM	1697	CZ	PHE	211	8.515	43.240	6.804	1.00	8.86
ATOM	1698	C	PHE	211	3.249	44.762	6.938	1.00	7.66
ATOM	1699	O	PHE	211	2.415	44.662	6.051	1.00	8.72
ATOM	1700	N	GLU	212	3.963	45.856	7.143	1.00	7.99
ATOM	1701	CA	GLU	212	3.752	47.072	6.365	1.00	7.78
ATOM	1702	CB	GLU	212	4.267	48.319	7.076	1.00	10.35
ATOM	1703	CG	GLU	212	3.201	49.142	7.809	1.00	15.96
ATOM	1704	CD	GLU	212	2.280	49.935	6.895	1.00	17.40
ATOM	1705	OE1	GLU	212	1.606	50.866	7.415	1.00	19.49
ATOM	1706	OE2	GLU	212	2.214	49.708	5.623	1.00	15.01
ATOM	1707	C	GLU	212	4.328	46.972	4.954	1.00	7.86
ATOM	1708	O	GLU	212	5.006	46.040	4.555	1.00	8.28
ATOM	1709	N	TRP	213	3.992	47.997	4.162	1.00	8.57
ATOM	1710	CA	TRP	213	4.464	48.141	2.806	1.00	8.31
ATOM	1711	CB	TRP	213	3.999	49.421	2.155	1.00	8.34
ATOM	1712	CG	TRP	213	4.620	50.707	2.603	1.00	9.80
ATOM	1713	CD2	TRP	213	5.776	51.317	2.074	1.00	11.28
ATOM	1714	CE2	TRP	213	5.977	52.520	2.784	1.00	12.37
ATOM	1715	CE3	TRP	213	6.644	50.973	1.031	1.00	12.51
ATOM	1716	CD1	TRP	213	4.181	51.522	3.610	1.00	10.15
ATOM	1717	NE1	TRP	213	4.980	52.619	3.734	1.00	12.18
ATOM	1718	CZ2	TRP	213	7.053	53.363	2.474	1.00	14.69
ATOM	1719	CZ3	TRP	213	7.687	51.805	0.735	1.00	13.88
ATOM	1720	CH2	TRP	213	7.887	52.990	1.460	1.00	15.53
ATOM	1721	C	TRP	213	5.991	48.089	2.741	1.00	7.51
ATOM	1722	O	TRP	213	6.720	48.548	3.592	1.00	8.44
ATOM	1723	N	HIS	214	6.470	47.422	1.657	1.00	7.74
ATOM	1724	CA	HIS	214	7.890	47.280	1.443	1.00	7.66
ATOM	1725	CB	HIS	214	8.495	46.246	2.447	1.00	7.45
ATOM	1726	CG	HIS	214	7.976	44.860	2.273	1.00	7.38
ATOM	1727	CD2	HIS	214	8.527	43.765	1.682	1.00	7.28
ATOM	1728	ND1	HIS	214	6.682	44.495	2.637	1.00	6.92
ATOM	1729	CE1	HIS	214	6.501	43.234	2.298	1.00	7.44
ATOM	1730	NE2	HIS	214	7.581	42.759	1.734	1.00	7.83
ATOM	1731	C	HIS	214	8.125	46.789	0.014	1.00	6.97
ATOM	1732	O	HIS	214	7.212	46.319	-0.642	1.00	7.95
ATOM	1733	N	GLU	215	9.384	46.910	-0.408	1.00	7.78
ATOM	1734	CA	GLU	215	9.921	46.226	-1.569	1.00	8.05
ATOM	1735	CB	GLU	215	10.780	47.140	-2.413	1.00	9.46
ATOM	1736	CG	GLU	215	10.056	48.276	-3.051	1.00	11.54
ATOM	1737	CD	GLU	215	10.919	49.189	-3.900	1.00	16.19
ATOM	1738	OE1	GLU	215	12.160	49.042	-3.934	1.00	15.97
ATOM	1739	OE2	GLU	215	10.349	50.051	-4.616	1.00	23.46
ATOM	1740	C	GLU	215	10.805	45.070	-1.025	1.00	8.11
ATOM	1741	O	GLU	215	11.385	45.184	0.071	1.00	8.95
ATOM	1742	N	ASP	216	10.913	43.985	-1.761	1.00	7.98
ATOM	1743	CA	ASP	216	11.723	42.873	-1.305	1.00	6.84
ATOM	1744	CB	ASP	216	11.363	41.564	-1.990	1.00	7.24
ATOM	1745	CG	ASP	216	10.037	40.991	-1.580	1.00	6.78
ATOM	1746	OD1	ASP	216	9.415	41.594	-0.693	1.00	7.44
ATOM	1747	OD2	ASP	216	9.648	39.909	-2.098	1.00	7.77
ATOM	1748	C	ASP	216	13.214	43.128	-1.469	1.00	6.24

ATOM	1749	O	ASP	216	13.696	43 704	-2 450	1.00	7.93
ATOM	1750	N	VAL	217	13.931	42.555	-0 509	1.00	6.61
ATOM	1751	CA	VAL	217	15 369	42 439	-0 559	1 00	6.71
ATOM	1752	CB	VAL	217	16.050	42.687	0.780	1 00	7.87
ATOM	1753	CG1	VAL	217	17 568	42.640	0.641	1 00	9.01
ATOM	1754	CG2	VAL	217	15 613	44.001	1.353	1 00	9.65
ATOM	1755	C	VAL	217	15.714	41.072	-1.150	1 00	6.75
ATOM	1756	O	VAL	217	15.769	40.051	-0 482	1.00	7.26
ATOM	1757	N	SER	218	15.852	41.047	-2 476	1.00	6.83
ATOM	1758	CA	SER	218	16.056	39.850	-3.257	1.00	6.43
ATOM	1759	CB	SER	218	14 837	38 910	-3 175	1.00	6.60
ATOM	1760	OG	SER	218	13.749	39.472	-3 890	1.00	6.81
ATOM	1761	C	SER	218	16.304	40.211	-4.722	1.00	5.92
ATOM	1762	O	SER	218	16.044	41.351	-5 112	1 00	6.97
ATOM	1763	N	LEU	219	16.723	39.209	-5.488	1.00	6.04
ATOM	1764	CA	LEU	219	16.663	39.294	-6.937	1.00	6.10
ATOM	1765	CB	LEU	219	17.722	38.393	-7.569	1.00	6.78
ATOM	1766	CG	LEU	219	17.728	38.321	-9.097	1.00	7.82
ATOM	1767	CD1	LEU	219	18.034	39 650	-9.731	1.00	9.76
ATOM	1768	CD2	LEU	219	18 660	37.225	-9.589	1.00	8.26
ATOM	1769	C	LEU	219	15.218	38.982	-7.341	1.00	5.92
ATOM	1770	O	LEU	219	14 541	39.784	-7.957	1.00	6.32
ATOM	1771	N	ILE	220	14 743	37.780	-6.965	1.00	5.60
ATOM	1772	CA	ILE	220	13.342	37.411	-7.010	1.00	5.79
ATOM	1773	CB	ILE	220	12.950	36 552	-8.228	1.00	6.51
ATOM	1774	CG2	ILE	220	13.285	37.295	-9.523	1.00	7.78
ATOM	1775	CG1	ILE	220	13.563	35.144	-8.189	1.00	6 95
ATOM	1776	CD1	ILE	220	13.002	34.222	-9.250	1.00	7.96
ATOM	1777	C	ILE	220	12.977	36.695	-5.712	1.00	5.16
ATOM	1778	O	ILE	220	13 869	36.252	-4.968	1.00	5.70
ATOM	1779	N	THR	221	11 694	36.656	-5.419	1.00	5.46
ATOM	1780	CA	THR	221	11.121	35.981	-4.263	1.00	6.07
ATOM	1781	CB	THR	221	10.391	36.988	-3.362	1.00	6.78
ATOM	1782	OG1	THR	221	11.360	37.970	-2.958	1.00	6 64
ATOM	1783	CG2	THR	221	9.809	36.316	-2.133	1.00	7.54
ATOM	1784	C	THR	221	10.182	34.891	-4.753	1.00	5 05
ATOM	1785	O	THR	221	9.365	35.121	-5.667	1.00	6 03
ATOM	1786	N	VAL	222	10.317	33.704	-4.181	1.00	5.43
ATOM	1787	CA	VAL	222	9.635	32.477	-4.589	1.00	5.29
ATOM	1788	CB	VAL	222	10.610	31.467	-5.188	1.00	5.74
ATOM	1789	CG1	VAL	222	9.950	30.168	-5.590	1.00	6 07
ATOM	1790	CG2	VAL	222	11.389	32.046	-6.358	1.00	6 22
ATOM	1791	C	VAL	222	8.867	31.924	-3.379	1.00	5.62
ATOM	1792	O	VAL	222	9.466	31.333	-2.465	1.00	5.72
ATOM	1793	N	LEU	223	7.572	32.200	-3.305	1.00	5.40
ATOM	1794	CA	LEU	223	6.799	32.054	-2.080	1.00	5 71
ATOM	1795	CB	LEU	223	6.211	33.454	-1.749	1.00	5.73
ATOM	1796	CG	LEU	223	5.245	33.563	-0.576	1.00	5.62
ATOM	1797	CD1	LEU	223	5.992	33.305	0.748	1 00	5 34
ATOM	1798	CD2	LEU	223	4.631	34.983	-0.564	1.00	7 58
ATOM	1799	C	LEU	223	5.672	31.053	-2.119	1.00	5 89
ATOM	1800	O	LEU	223	4.853	31.106	-3.012	1.00	6.54
ATOM	1801	N	TYR	224	5.637	30.185	-1.112	1.00	5.35
ATOM	1802	CA	TYR	224	4.493	29.307	-0.858	1.00	5 93
ATOM	1803	CB	TYR	224	4.891	27.865	-0.543	1.00	7.37
ATOM	1804	CG	TYR	224	3.696	27.082	-0 030	1.00	8 60
ATOM	1805	CD1	TYR	224	2.805	26.474	-0.888	1.00	10 86
ATOM	1806	CE1	TYR	224	1.698	25.762	-0.350	1.00	11 92
ATOM	1807	CD2	TYR	224	3.459	26.927	1 341	1.00	10.88
ATOM	1808	CE2	TYR	224	2.363	26.334	1 897	1.00	12 37
ATOM	1809	CZ	TYR	224	1 500	25.717	1 012	1.00	12 52
ATOM	1810	OH	TYR	224	0 388	25.081	1 575	1.00	16.93
ATOM	1811	C	TYR	224	3 702	29.956	0 284	1.00	5 19
ATOM	1812	O	TYR	224	4 318	30.259	1 319	1.00	6 49
ATOM	1813	N	GLN	225	2 391	29.993	0 209	1.00	5 70
ATOM	1814	CA	GLN	225	1 552	30.327	1 336	1.00	6 51
ATOM	1815	CB	GLN	225	1.053	31.753	1 362	1.00	8 15
ATOM	1816	CG	GLN	225	2.113	32.840	1.196	1.00	8 18
ATOM	1817	CD	GLN	225	1.591	34.205	1 582	1.00	8.60
ATOM	1818	OE1	GLN	225	2.147	34.911	2 439	1.00	11 27
ATOM	1819	NE2	GLN	225	0.536	34.580	0 927	1.00	9.01
ATOM	1820	C	GLN	225	0.332	29.411	1 366	1.00	7.75
ATOM	1821	O	GLN	225	-0.163	28.937	0 352	1.00	8.52

ATOM	1822	N	SER	226	-0.198	29.227	2.575	1.00	9.34
ATOM	1823	CA	SER	226	-1.464	28.544	2.758	1.00	10.96
ATOM	1824	CB	SER	226	-2.003	28.665	4.164	1.00	16.30
ATOM	1825	OG	SER	226	-1.115	28.419	5.120	1.00	15.06
ATOM	1826	C	SER	226	-2.559	29.310	2.014	1.00	10.35
ATOM	1827	O	SER	226	-2.481	30.484	1.699	1.00	11.80
ATOM	1828	N	ASN	227	-3.684	28 605	1.934	1.00	10.66
ATOM	1829	CA	ASN	227	-4.840	29 105	1.234	1.00	11.50
ATOM	1830	CB	ASN	227	-5.725	27 953	0.769	1.00	15.38
ATOM	1831	CG	ASN	227	-6.303	28.312	-0.576	1.00	22.10
ATOM	1832	OD1	ASN	227	-6.033	27.643	-1.583	1.00	35.45
ATOM	1833	ND2	ASN	227	-6.869	29.471	-0.713	1.00	20.67
ATOM	1834	C	ASN	227	-5 668	30.072	2.070	1.00	12.61
ATOM	1835	O	ASN	227	-6 857	29.812	2.296	1.00	15.01
ATOM	1836	N	VAL	228	-5 078	31.162	2.514	1.00	10.77
ATOM	1837	CA	VAL	228	-5 746	32.223	3.268	1.00	9.90
ATOM	1838	CB	VAL	228	-5 417	32.224	4.768	1.00	11.72
ATOM	1839	CG1	VAL	228	-6 173	33.357	5.454	1.00	14.80
ATOM	1840	CG2	VAL	228	-5.721	30.872	5.403	1.00	14.80
ATOM	1841	C	VAL	228	-5 284	33.531	2.644	1.00	9.82
ATOM	1842	O	VAL	228	-4 093	33.821	2.657	1.00	10.96
ATOM	1843	N	GLN	229	-6 185	34.288	2.031	1.00	9.94
ATOM	1844	CA	GLN	229	-5 815	35.512	1.345	1.00	9.11
ATOM	1845	CB	GLN	229	-7 038	36.050	0.595	1.00	10.74
ATOM	1846	CG	GLN	229	-6 750	37.084	-0.481	1.00	10.34
ATOM	1847	CD	GLN	229	-6 454	38.479	0.038	1.00	11.49
ATOM	1848	OE1	GLN	229	-7 057	38.953	1.011	1.00	12.74
ATOM	1849	NE2	GLN	229	-5.440	39.124	-0.556	1.00	10.77
ATOM	1850	C	GLN	229	-5.228	36.489	2.340	1 00	9.22
ATOM	1851	O	GLN	229	-5.784	36.712	3.421	1 00	10.98
ATOM	1852	N	ASN	230	-4.133	37.140	1.924	1 00	8.54
ATOM	1853	CA	ASN	230	-3.504	38.106	2.839	1 00	9.75
ATOM	1854	CB	ASN	230	-2.642	37.356	3.865	1 00	10.52
ATOM	1855	CG	ASN	230	-1.468	36.649	3.229	1 00	11.42
ATOM	1856	OD1	ASN	230	-1.601	35.602	2.559	1.00	12.95
ATOM	1857	ND2	ASN	230	-0.321	37.258	3.367	1 00	10.36
ATOM	1858	C	ASN	230	-2 684	39.177	2.186	1.00	9.22
ATOM	1859	O	ASN	230	-2 579	40.278	2.699	1 00	10.88
ATOM	1860	N	LEU	231	-2 080	38.928	1.008	1 00	8.35
ATOM	1861	CA	LEU	231	-1 187	39.891	0.391	1 00	7.65
ATOM	1862	CB	LEU	231	-0 166	39.130	-0.486	1.00	9.10
ATOM	1863	CG	LEU	231	0 859	38.294	0.253	1 00	10.43
ATOM	1864	CD1	LEU	231	1.718	37.494	-0 719	1.00	12.85
ATOM	1865	CD2	LEU	231	1 707	39.142	1.167	1.00	18.74
ATOM	1866	C	LEU	231	-1 921	40.933	-0.444	1.00	7.60
ATOM	1867	O	LEU	231	-2 902	40.618	-1.110	1.00	8.69
ATOM	1868	N	GLN	232	-1 378	42.167	-0.446	1.00	7.25
ATOM	1869	CA	GLN	232	-1 884	43.212	-1.298	1.00	7.79
ATOM	1870	CB	GLN	232	-2.611	44.274	-0.523	1.00	8.77
ATOM	1871	CG	GLN	232	-3.852	43.777	0.218	1.00	8.38
ATOM	1872	CD	GLN	232	-4.616	44.915	0.825	1.00	10.24
ATOM	1873	OE1	GLN	232	-4.059	45.793	1.487	1.00	11.66
ATOM	1874	NE2	GLN	232	-5.935	44.904	0 648	1.00	14.46
ATOM	1875	C	GLN	232	-0.682	43.819	-2 003	1.00	6.81
ATOM	1876	O	GLN	232	0.375	43.965	-1.390	1.00	7.95
ATOM	1877	N	VAL	233	-0.905	44.246	-3 244	1.00	7.92
ATOM	1878	CA	VAL	233	0.087	44.893	-4 061	1.00	8.46
ATOM	1879	CB	VAL	233	0.462	44.130	-5 339	1.00	9.34
ATOM	1880	CG1	VAL	233	-0.719	43.775	-6.224	1.00	10.46
ATOM	1881	CG2	VAL	233	1.534	44.837	-6.141	1.00	9.44
ATOM	1882	C	VAL	233	-0.381	46.307	-4.399	1.00	8.77
ATOM	1883	O	VAL	233	-1.556	46.486	-4.737	1.00	10.72
ATOM	1884	N	GLU	234	0.489	47.302	-4.314	1.00	8.62
ATOM	1885	CA	GLU	234	0.169	48.654	-4.763	1.00	10.41
ATOM	1886	CB	GLU	234	1.095	49.693	-4.115	1.00	11.08
ATOM	1887	CG	GLU	234	0 638	51.126	-4.319	1.00	12.76
ATOM	1888	CD	GLU	234	1.488	52 093	-3.531	1.00	13.73
ATOM	1889	OE1	GLU	234	2.730	51.975	-3.567	1.00	16.36
ATOM	1890	OE2	GLU	234	0.903	53 025	-2.925	1.00	16.64
ATOM	1891	C	GLU	234	0.277	48.736	-6.285	1.00	12.14
ATOM	1892	O	GLU	234	1.295	48.366	-6.885	1.00	13.51
ATOM	1893	N	THR	235	-0.753	49.285	-6.917	1.00	15.59
ATOM	1894	CA	THR	235	-0.699	49.507	-8.364	1.00	17.29

ATOM	1895	CB	THR	235	-1.595	48 591	-9.200	1 00	19 13
ATOM	1896	OG1	THR	235	-2.984	48 842	-8.938	1 00	21 58
ATOM	1897	CG2	THR	235	-1 375	47 100	-8.952	1.00	22 36
ATOM	1898	C	THR	235	-1 137	50 959	-8.576	1 00	18 85
ATOM	1899	O	THR	235	-1 394	51.656	-7.579	1 00	19.19
ATOM	1900	N	ALA	236	-1.293	51.330	-9.856	1 00	22 89
ATOM	1901	CA	ALA	236	-1.784	52 664	-10.222	1 00	23 88
ATOM	1902	CB	ALA	236	-1 749	52 884	-11.725	1.00	31 13
ATOM	1903	C	ALA	236	-3.206	52.889	-9.731	1.00	24 49
ATOM	1904	O	ALA	236	-3.723	53.962	-9.427	1.00	31.36
ATOM	1905	N	ALA	237	-3.929	51.774	-9.619	1.00	24.56
ATOM	1906	CA	ALA	237	-5.299	51 889	-9.150	1 00	25.87
ATOM	1907	CB	ALA	237	-6.155	50 804	-9.815	1.00	33.93
ATOM	1908	C	ALA	237	-5 332	51.715	-7 648	1.00	24.45
ATOM	1909	O	ALA	237	-6 424	51.484	-7 120	1 00	30.47
ATOM	1910	N	GLY	238	-4.223	51.758	-6 932	1.00	21.71
ATOM	1911	CA	GLY	238	-4.269	51.563	-5 481	1.00	19.83
ATOM	1912	C	GLY	238	-3.842	50.185	-5 013	1.00	17.46
ATOM	1913	O	GLY	238	-3.387	49.372	-5.837	1.00	17.96
ATOM	1914	N	TYR	239	-4 061	49 844	-3.728	1.00	15.86
ATOM	1915	CA	TYR	239	-3 721	48.501	-3.275	1.00	12.97
ATOM	1916	CB	TYR	239	-3.579	48.458	-1.743	1.00	12.30
ATOM	1917	CG	TYR	239	-2.235	48 936	-1.252	1.00	11.99
ATOM	1918	CD1	TYR	239	-2 034	50 267	-0.939	1.00	12.25
ATOM	1919	CE1	TYR	239	-0 787	50 701	-0.501	1.00	12.55
ATOM	1920	CD2	TYR	239	-1.161	48 056	-1.168	1.00	11.54
ATOM	1921	CE2	TYR	239	0.072	48 470	-0.746	1.00	11.38
ATOM	1922	CZ	TYR	239	0.238	49.811	-0.426	1.00	11.23
ATOM	1923	OH	TYR	239	1.484	50.235	-0.015	1.00	14.40
ATOM	1924	C	TYR	239	-4.815	47.516	-3.705	1.00	12.53
ATOM	1925	O	TYR	239	-6.007	47.800	-3.513	1.00	17.24
ATOM	1926	N	GLN	240	-4.409	46.398	-4.296	1.00	11.52
ATOM	1927	CA	GLN	240	-5.297	45.349	-4.769	1.00	11.73
ATOM	1928	CB	GLN	240	-5.117	45.199	-6.306	1.00	11.64
ATOM	1929	CG	GLN	240	-5.539	46.485	-7.051	1.00	14.46
ATOM	1930	CD	GLN	240	-5.418	46.379	-8.546	1.00	16.63
ATOM	1931	OE1	GLN	240	-4.585	45.635	-9.069	1.00	18.79
ATOM	1932	NE2	GLN	240	-6.217	47.136	-9.296	1.00	21.51
ATOM	1933	C	GLN	240	-4.935	44.026	-4.113	1.00	10.88
ATOM	1934	O	GLN	240	-3.763	43.770	-3.789	1.00	9.92
ATOM	1935	N	ASP	241	-5.922	43.182	-3.859	1.00	10.67
ATOM	1936	CA	ASP	241	-5.711	41.915	-3.230	1.00	9.82
ATOM	1937	CB	ASP	241	-7.072	41.409	-2.727	1.00	11.01
ATOM	1938	CG	ASP	241	-7.532	41.987	-1.420	1.00	12.59
ATOM	1939	OD1	ASP	241	-8.763	41.911	-1.141	1.00	15.81
ATOM	1940	OD2	ASP	241	-6.719	42.478	-0.648	1.00	12.84
ATOM	1941	C	ASP	241	-5.124	40.876	-4.183	1.00	10.03
ATOM	1942	O	ASP	241	-5.613	40.615	-5.276	1.00	13.99
ATOM	1943	N	ILE	242	-4.082	40.170	-3.742	1.00	8.45
ATOM	1944	CA	ILE	242	-3.524	39.035	-4.454	1.00	8.44
ATOM	1945	CB	ILE	242	-2.024	38.896	-4.197	1.00	8.68
ATOM	1946	CG2	ILE	242	-1.499	37.564	-4.760	1.00	10.88
ATOM	1947	CG1	ILE	242	-1.271	40.096	-4.766	1.00	9.70
ATOM	1948	CD1	ILE	242	0.191	40.223	-4.344	1.00	11.78
ATOM	1949	C	ILE	242	-4.242	37.784	-3.942	1.00	8.96
ATOM	1950	O	ILE	242	-4.216	37.474	-2.740	1.00	9.65
ATOM	1951	N	ALA	243	-4.926	37.054	-4.821	1.00	9.75
ATOM	1952	CA	ALA	243	-5 595	35.814	-4.414	1.00	9.73
ATOM	1953	C	ALA	243	-4.574	34.776	-3.950	1.00	8.94
ATOM	1954	O	ALA	243	-3 463	34.685	-4.478	1.00	11.10
ATOM	1955	CB	ALA	243	-6.379	35.243	-5.605	1.00	14.74
ATOM	1956	N	ALA	244	-4 991	33.948	-2 985	1.00	9.36
ATOM	1957	CA	ALA	244	-4 136	32.844	-2 547	1.00	9.36
ATOM	1958	CB	ALA	244	-4.588	32.409	-1 156	1.00	13.93
ATOM	1959	C	ALA	244	-4.243	31.707	-3.540	1.00	10.49
ATOM	1960	O	ALA	244	-5.263	31 547	-4 224	1.00	13.13
ATOM	1961	N	ASP	245	-3.215	30 899	-3 615	1.00	10.92
ATOM	1962	CA	ASP	245	-3.158	29 661	-4 408	1.00	11.37
ATOM	1963	CB	ASP	245	-2.804	29 876	-5.858	1.00	11 89
ATOM	1964	CG	ASP	245	-2.892	28.664	-6.747	1.00	13 54
ATOM	1965	OD1	ASP	245	-3.031	28.761	-7.996	1.00	18 77
ATOM	1966	OD2	ASP	245	-2.886	27.549	-6.197	1.00	13.74
ATOM	1967	C	ASP	245	-2.109	28.779	-3.720	1.00	10.46

ATOM	1968	O	ASP	245	-0.917	28.912	-3.998	1.00	11.30
ATOM	1969	N	ASP	246	-2.562	27.850	-2.905	1.00	9.06
ATOM	1970	CA	ASP	246	-1.677	26.921	-2.197	1.00	9.74
ATOM	1971	CB	ASP	246	-2.253	26.499	-0.859	1.00	11.33
ATOM	1972	CG	ASP	246	-3 378	25.495	-1.011	1.00	13.92
ATOM	1973	OD1	ASP	246	-3 834	24.958	0.018	1.00	15.40
ATOM	1974	OD2	ASP	246	-3 870	25.292	-2.155	1 00	14.85
ATOM	1975	C	ASP	246	-1.201	25.755	-3.060	1.00	9.71
ATOM	1976	O	ASP	246	-0.571	24.838	-2.544	1 00	10 59
ATOM	1977	N	THR	247	-1 417	25 840	-4.379	1.00	9 46
ATOM	1978	CA	THR	247	-0 834	24 865	-5.261	1 00	9 37
ATOM	1979	CB	THR	247	-1 845	24 275	-6.269	1 00	11 29
ATOM	1980	OG1	THR	247	-2 235	25 290	-7.212	1.00	11 39
ATOM	1981	CG2	THR	247	-3 094	23 800	-5.524	1 00	12 30
ATOM	1982	C	THR	247	0 328	25 442	-6.058	1 00	8 75
ATOM	1983	O	THR	247	1 026	24 639	-6.698	1.00	11.70
ATOM	1984	N	GLY	248	0.477	26.744	-6.088	1 00	8.16
ATOM	1985	CA	GLY	248	1.475	27.454	-6 872	1.00	8.63
ATOM	**1986**	**C**	**GLY**	**248**	**2.494**	**28.172**	**-5.992**	**1.00**	**7.49**
ATOM	1987	O	GLY	248	2.373	28.246	-4.757	1.00	10.66
ATOM	1988	N	TYR	249	3.496	28.733	-6 663	1.00	6.67
ATOM	1989	CA	TYR	249	4.437	29.616	-6.005	1.00	6 51
ATOM	1990	CB	TYR	249	5 900	29 244	-6.303	1 00	6 70
ATOM	1991	CG	TYR	249	6.411	28 129	-5.426	1.00	6 10
ATOM	1992	CD1	TYR	249	6 314	26 788	-5 752	1.00	6 62
ATOM	1993	CE1	TYR	249	6.786	25.803	-4 929	1 00	7 14
ATOM	1994	CD2	TYR	249	6 992	28 437	-4.199	1 00	5 64
ATOM	1995	CE2	TYR	249	7.470	27.450	-3.364	1.00	5.23
ATOM	1996	CZ	TYR	249	7.367	26.135	-3.715	1 00	6.30
ATOM	1997	OH	TYR	249	7 823	25.130	-2.903	1 00	8 55
ATOM	1998	C	TYR	249	4 202	31.046	-6.523	1 00	5.67
ATOM	1999	O	TYR	249	4.146	31.252	-7.740	1.00	6 93
ATOM	2000	N	LEU	250	4.045	31.976	-5 592	1.00	5 56
ATOM	2001	CA	LEU	250	3.894	33.381	-5.926	1.00	5 35
ATOM	2002	CB	LEU	250	3.151	34.119	-4 803	1.00	6.61
ATOM	2003	CG	LEU	250	2.830	35.587	-5.134	1.00	6 78
ATOM	2004	CD1	LEU	250	1.810	35.727	-6 251	1.00	7 40
ATOM	2005	CD2	LEU	250	2 316	36.240	-3.857	1.00	8.54
ATOM	2006	C	LEU	250	5.283	33.945	-6.147	1.00	5 86
ATOM	2007	O	LEU	250	6 157	33.797	-5.272	1 00	5 91
ATOM	2008	N	ILE	251	5.498	34.540	-7.312	1.00	5 45
ATOM	2009	CA	ILE	251	6 777	35.088	-7.727	1 00	6 03
ATOM	2010	CB	ILE	251	7.240	34.434	-9.059	1 00	6 08
ATOM	2011	CG2	ILE	251	8 728	34.801	-9.306	1.00	7.80
ATOM	2012	CG1	ILE	251	6.975	32.941	-9.095	1 00	5.58
ATOM	2013	CD1	ILE	251	7.657	32.110	-8.038	1.00	6.65
ATOM	2014	C	ILE	251	6 712	36.599	-7.909	1 00	6.10
ATOM	2015	O	ILE	251	5 735	37.111	-8.484	1 00	6.96
ATOM	2016	N	ASN	252	7.760	37.291	-7.443	1 00	6.11
ATOM	2017	CA	ASN	252	7.892	38.703	-7.696	1 00	6.61
ATOM	2018	CB	ASN	252	7.145	39.615	-6.739	1 00	7.62
ATOM	2019	CG	ASN	252	7.617	39 521	-5.306	1 00	8.27
ATOM	2020	OD1	ASN	252	7.166	38 626	-4.587	1 00	9 37
ATOM	2021	ND2	ASN	252	8.520	40.387	-4.902	1 00	8 45
ATOM	2022	C	ASN	252	9.377	39 065	-7.731	1 00	6 35
ATOM	2023	O	ASN	252	10.197	38 345	-7.137	1.00	7 21
ATOM	2024	N	CYS	253	9.683	40.236	-8.295	1.00	6 40
ATOM	2025	CA	CYS	253	11.048	40.768	-8.285	1.00	7 03
ATOM	2026	CB	CYS	253	11.302	41.723	-9.464	1.00	8 85
ATOM	2027	SG	CYS	253	11.232	40.881	-11.077	1.00	10 36
ATOM	2028	C	CYS	253	11.309	41.552	-6.988	1.00	7 30
ATOM	2029	O	CYS	253	10.402	42.203	-6.420	1.00	7 55
ATOM	2030	N	GLY	254	12.562	41.539	-6.585	1.00	6 67
ATOM	2031	CA	GLY	254	13.063	42.360	-5.503	1.00	7 05
ATOM	2032	C	GLY	254	13.850	43.536	-6.046	1.00	7.09
ATOM	2033	O	GLY	254	14.011	43.696	-7.269	1.00	7.78
ATOM	2034	N	SER	255	14.338	44.380	-5.130	1.00	7.39
ATOM	2035	CA	SER	255	14.942	45.634	-5.560	1.00	8.33
ATOM	2036	CB	SER	255	14.980	46.646	-4.420	1.00	8.09
ATOM	2037	OG	SER	255	15.785	46.124	-3.385	1.00	9.54
ATOM	2038	C	SER	255	16 275	45.443	-6.277	1.00	7.85
ATOM	2039	O	SER	255	16 710	46.348	-6.979	1.00	10.10
ATOM	2040	N	TYR	256	16.928	44.287	-6.184	1.00	7.83

ATOM	2041	CA	TYR	256	18.151	44.106	-6.964	1.00	8.12
ATOM	2042	CB	TYR	256	18 966	42.909	-6.486	1.00	7.96
ATOM	2043	CG	TYR	256	20 395	42.919	-7 017	1.00	7 92
ATOM	2044	CD1	TYR	256	21.351	43.735	-6 425	1.00	9.18
ATOM	2045	CE1	TYR	256	22 665	43.731	-6.866	1.00	9 56
ATOM	2046	CD2	TYR	256	20.800	42.110	-8 068	1.00	8 38
ATOM	2047	CE2	TYR	256	22.119	42.114	-8 530	1.00	8 77
ATOM	2048	CZ	TYR	256	23 030	42 931	-7.942	1.00	7 91
ATOM	2049	OH	TYR	256	24 334	42.919	-8 446	1.00	10 55
ATOM	2050	C	TYR	256	17.790	44.007	-8.444	1.00	7 77
ATOM	2051	O	TYR	256	18 510	44.559	-9 307	1.00	9.14
ATOM	2052	N	MET	257	16 689	43.310	-8 767	1.00	8.12
ATOM	2053	CA	MET	257	16 220	43 230	-10.151	1.00	7.70
ATOM	2054	CB	MET	257	15.002	42.301	-10.305	1.00	8 40
ATOM	2055	CG	MET	257	14.582	42 102	-11.738	1.00	9 02
ATOM	2056	SD	MET	257	15.730	41 115	-12.738	1.00	9 56
ATOM	2057	CE	MET	257	15.233	39 485	-12.131	1.00	11.37
ATOM	2058	C	MET	257	15.843	44.629	-10 670	1.00	6 94
ATOM	2059	O	MET	257	16.150	44.976	-11.819	1.00	8.48
ATOM	2060	N	ALA	258	15.189	45.427	-9.842	1.00	7.83
ATOM	2061	CA	ALA	258	14.807	46.786	-10.242	1.00	8.49
ATOM	2062	CB	ALA	258	13.940	47.433	-9.204	1.00	8.60
ATOM	2063	C	ALA	258	16.074	47 582	-10.550	1.00	8.95
ATOM	2064	O	ALA	258	16.128	48.339	-11 526	1.00	10 68
ATOM	2065	N	HIS	259	17.075	47.456	-9 717	1.00	9 55
ATOM	2066	CA	HIS	259	18.325	48.184	-9 987	1.00	9 84
ATOM	2067	CB	HIS	259	19.298	47.968	-8.806	1.00	10.82
ATOM	2068	CG	HIS	259	20.581	48.672	-8.960	1.00	12.01
ATOM	2069	CD2	HIS	259	20.785	50.004	-8.919	1.00	11.84
ATOM	2070	ND1	HIS	259	21.801	48.079	-9.209	1.00	14.52
ATOM	2071	CE1	HIS	259	22.701	49.050	-9.270	1.00	12.90
ATOM	2072	NE2	HIS	259	22.106	50.209	-9.115	1.00	14.66
ATOM	2073	C	HIS	259	18.949	47.746	-11.296	1.00	9.17
ATOM	2074	O	HIS	259	19.275	48.580	-12.144	1.00	11.20
ATOM	2075	N	LEU	260	19.091	46.450	-11.529	1.00	9.71
ATOM	2076	CA	LEU	260	19.763	45.917	-12.699	1.00	11.16
ATOM	2077	CB	LEU	260	19.771	44.362	-12.647	1.00	13.64
ATOM	2078	CG	LEU	260	20.621	43.697	-11.579	1.00	14.53
ATOM	2079	CD1	LEU	260	20.446	42.195	-11.659	1.00	15.33
ATOM	2080	CD2	LEU	260	22.081	44.131	-11.700	1.00	18.49
ATOM	2081	C	LEU	260	19.044	46.315	-13.989	1.00	10.90
ATOM	2082	O	LEU	260	19.715	46.435	-15.017	1.00	11.94
ATOM	2083	N	THR	261	17.723	46.442	-13.932	1.00	9.82
ATOM	2084	CA	THR	261	16.920	46.680	-15.141	1.00	10.23
ATOM	2085	CB	THR	261	15.671	45.798	-15.202	1.00	9.32
ATOM	2086	OG1	THR	261	14.737	46.138	-14.174	1.00	9.59
ATOM	2087	CG2	THR	261	16.000	44.325	-15.098	1.00	10.96
ATOM	2088	C	THR	261	16.492	48.151	-15.298	1.00	10.83
ATOM	2089	O	THR	261	15.664	48.493	-16.138	1.00	12.22
ATOM	2090	N	ASN	262	17.009	48.999	-14.417	1.00	12.86
ATOM	2091	CA	ASN	262	16.643	50.411	-14.405	1.00	13.99
ATOM	2092	CB	ASN	262	17.162	51.124	-15.670	1.00	16.72
ATOM	2093	CG	ASN	262	17.122	52 624	-15.414	1.00	18.91
ATOM	2094	OD1	ASN	262	17.484	53 032	-14.306	1.00	23.20
ATOM	2095	ND2	ASN	262	16.604	53 423	-16.351	1.00	23.32
ATOM	2096	C	ASN	262	15.143	50 639	-14.281	1.00	14.56
ATOM	2097	O	ASN	262	14.524	51.455	-14.945	1.00	17.11
ATOM	2098	N	ASN	263	14.570	49 836	-13.381	1.00	13.82
ATOM	2099	CA	ASN	263	13.148	49 902	-13.081	1.00	15.46
ATOM	2100	CB	ASN	263	12 863	51.289	-12.502	1.00	17.97
ATOM	2101	CG	ASN	263	12.214	51.276	-11.157	1.00	17.06
ATOM	2102	OD1	ASN	263	12 128	50.271	-10.466	1.00	15.00
ATOM	2103	ND2	ASN	263	11.533	52 359	-10.866	1.00	25.64
ATOM	2104	C	ASN	263	12.252	49 450	-14.215	1.00	13.77
ATOM	2105	O	ASN	263	11 012	49 566	-14.160	1.00	18.41
ATOM	2106	N	TYR	264	12 774	48 764	-15.236	1.00	13.79
ATOM	2107	CA	TYR	264	11 900	48 149	-16.255	1.00	14.19
ATOM	2108	CB	TYR	264	12.715	47 613	-17.416	1.00	15.13
ATOM	2109	CG	TYR	264	11 996	46 818	-18.494	1.00	16.36
ATOM	2110	CD1	TYR	264	11 035	47 371	-19 362	1.00	17.78
ATOM	2111	CE1	TYR	264	10 400	46.634	-20.350	1.00	18.06
ATOM	2112	CD2	TYR	264	12.259	45.484	-18.745	1.00	16.68
ATOM	2113	CE2	TYR	264	11.650	44.748	-19.760	1.00	16.65

ATOM	2114	CZ	TYR	264	10.716	45.314	-20.586	1.00	18.96
ATOM	2115	OH	TYR	264	10.037	44.587	-21.573	1.00	18.75
ATOM	2116	C	TYR	264	11.078	47.051	-15.593	1.00	12.40
ATOM	2117	O	TYR	264	9.880	46.958	-15.851	1.00	13.61
ATOM	2118	N	TYR	265	11.724	46.245	-14.738	1.00	10.62
ATOM	2119	CA	TYR	265	11.038	45.308	-13.845	1.00	9.32
ATOM	2120	CB	TYR	265	11.580	43.896	-13.877	1 00	9.65
ATOM	2121	CG	TYR	265	11.384	43.145	-15.197	1 00	9.18
ATOM	2122	CD1	TYR	265	11.979	41 897	-15.374	1 00	9.12
ATOM	2123	CE1	TYR	265	11 788	41 151	-16.513	1 00	9.35
ATOM	2124	CD2	TYR	265	10 575	43.607	-16.232	1 00	9.97
ATOM	2125	CE2	TYR	265	10 412	42 861	-17.391	1 00	9.60
ATOM	2126	CZ	TYR	265	11 019	41 653	-17.546	1 00	8.98
ATOM	2127	OH	TYR	265	10 956	40.929	-18 694	1 00	9.24
ATOM	2128	C	TYR	265	11 143	45 898	-12 455	1 00	8.87
ATOM	2129	O	TYR	265	12 165	45 736	-11.793	1 00	10 25
ATOM	2130	N	LYS	266	10 091	46 591	-12 039	1 00	9 35
ATOM	2131	CA	LYS	266	10 042	47 206	-10 722	1.00	10 27
ATOM	2132	CB	LYS	266	8.764	48.067	-10 642	1.00	11.78
ATOM	2133	CG	LYS	266	8.798	49.269	-11.544	1 00	15 74
ATOM	2134	CD	LYS	266	7.679	50.219	-11.609	1 00	20 41
ATOM	2135	CE	LYS	266	8 060	51 436	-12.461	1.00	27 25
ATOM	2136	NZ	LYS	266	8 880	51 073	-13 684	1 00	38 27
ATOM	2137	C	LYS	266	9 917	46.141	-9.642	1 00	9 64
ATOM	2138	O	LYS	266	9 483	45 006	-9 859	1 00	11 23
ATOM	2139	N	ALA	267	10 398	46 485	-8 457	1 00	8 21
ATOM	2140	CA	ALA	267	10 177	45.669	-7 302	1 00	8.00
ATOM	2141	CB	ALA	267	11.263	45 935	-6 279	1 00	9.27
ATOM	2142	C	ALA	267	8 810	46.112	-6 747	1 00	8.06
ATOM	2143	O	ALA	267	8 703	47 252	-6.265	1.00	9 31
ATOM	2144	N	PRO	268	7.786	45.314	-6.903	1 00	7 87
ATOM	2145	CD	PRO	268	7.704	43 960	-7 464	1 00	8.45
ATOM	2146	CA	PRO	268	6 464	45.815	-6.507	1.00	8.53
ATOM	2147	CB	PRO	268	5.497	44.732	-6.971	1 00	8 95
ATOM	2148	CG	PRO	268	6 340	43 491	-6.981	1.00	9.67
ATOM	2149	C	PRO	268	6.342	46 060	-5.020	1 00	7.51
ATOM	2150	O	PRO	268	6 832	45 247	-4 237	1.00	8.65
ATOM	2151	N	ILE	269	5 648	47 157	-4.658	1 00	7.63
ATOM	2152	CA	ILE	269	5 356	47 441	-3.254	1.00	7.94
ATOM	2153	CB	ILE	269	5 120	48 928	-2.981	1.00	9 79
ATOM	2154	CG2	ILE	269	4 494	49 172	-1.634	1 00	10 56
ATOM	2155	CG1	ILE	269	6 437	49.720	-3.185	1.00	13 68
ATOM	2156	CD1	ILE	269	6.187	51 182	-3.479	1.00	23.32
ATOM	2157	C	ILE	269	4.170	46.593	-2.837	1.00	7 83
ATOM	2158	O	ILE	269	3.149	46 540	-3.511	1.00	9 16
ATOM	2159	N	HIS	270	4 317	45.894	-2.703	1.00	7 29
ATOM	2160	CA	HIS	270	3 276	45 019	-2.206	1.00	7 01
ATOM	2161	CB	HIS	270	3.400	43.626	-1.835	1.00	7 25
ATOM	2162	CG	HIS	270	4.744	43.024	-1.598	1.00	7 13
ATOM	2163	CD2	HIS	270	5 128	42.038	-0.746	1.00	7 31
ATOM	2164	ND1	HIS	270	5 880	43.389	-2.273	1.00	7 07
ATOM	2165	CE1	HIS	270	6 904	42.683	-1.826	1.00	7 87
ATOM	2166	NE2	HIS	270	6.489	41.831	-0.890	1.00	7 31
ATOM	2167	C	HIS	270	3.274	44.991	0.302	1.00	6 54
ATOM	2168	O	HIS	270	4.212	45.458	0.936	1.00	7 63
ATOM	2169	N	ARG	271	2.201	44.490	0.896	1.00	6.78
ATOM	2170	CA	ARG	271	1.988	44.467	2.318	1.00	6.60
ATOM	2171	CB	ARG	271	1.366	45.769	2.853	1.00	7.26
ATOM	2172	CG	ARG	271	-0.088	45.972	2.398	1.00	8.12
ATOM	2173	CD	ARG	271	-0.543	47.381	2.652	1.00	8.48
ATOM	2174	NE	ARG	271	-1.974	47.504	2.297	1.00	9.27
ATOM	2175	CZ	ARG	271	-2.643	48.651	2.312	1.00	9.64
ATOM	2176	NH1	ARG	271	-2.060	49.802	2.648	1.00	10.45
ATOM	2177	NH2	ARG	271	-3.930	48.660	1.968	1.00	11.63
ATOM	2178	C	ARG	271	1.144	43.252	2.682	1.00	6.79
ATOM	2179	O	ARG	271	0.517	42.637	1.805	1.00	7.95
ATOM	2180	N	VAL	272	1.154	42.887	3.953	1.00	7.39
ATOM	2181	CA	VAL	272	0.444	41.736	4.493	1.00	6.97
ATOM	2182	CB	VAL	272	1.369	40.830	5.328	1.00	7.37
ATOM	2183	CG1	VAL	272	0.615	39.661	5.865	1.00	9.31
ATOM	2184	CG2	VAL	272	2.609	40.388	4.562	1.00	9.68
ATOM	2185	C	VAL	272	-0.712	42.173	5.378	1.00	6.78
ATOM	2186	O	VAL	272	-0.470	42.805	6.415	1.00	7.67

ATOM	2187	N	LYS	273	-1 917	41.839	4 950	1.00	7 33
ATOM	2188	CA	LYS	273	-3.061	42.135	5 792	1 00	8 38
ATOM	2189	CB	LYS	273	-4 364	41.763	5 047	1 00	9 72
ATOM	2190	CG	LYS	273	-4 658	42.765	3 950	1.00	13 66
ATOM	2191	CD	LYS	273	-6 090	42 725	3 437	1.00	20.08
ATOM	2192	CE	LYS	273	-6 381	41 379	2 873	1.00	21.66
ATOM	2193	NZ	LYS	273	-7 801	41 227	2.413	1 00	19.22
ATOM	2194	C	LYS	273	-3 047	41 256	7 047	1.00	7.72
ATOM	2195	O	LYS	273	-2.628	40 112	7 023	1 00	8.06
ATOM	2196	N	TRP	274	-3.644	41.812	8 114	1 00	7.85
ATOM	2197	CA	TRP	274	-3.914	41 041	9 322	1 00	8 01
ATOM	2198	CB	TRP	274	-4.314	41 953	10.481	1.00	8 38
ATOM	2199	CG	TRP	274	-4 864	41.210	11 655	1.00	8 22
ATOM	2200	CD2	TRP	274	-6 226	41.225	12 078	1.00	8.59
ATOM	2201	CE2	TRP	274	-6.311	40 370	13 188	1.00	9.28
ATOM	2202	CE3	TRP	274	-7.393	41 859	11 630	1 00	10.81
ATOM	2203	CD1	TRP	274	-4.216	40.377	12.490	1 00	8 98
ATOM	2204	NE1	TRP	274	-5 074	39.850	13.430	1 00	9 16
ATOM	2205	CZ2	TRP	274	-7 485	40.145	13.881	1.00	9 84
ATOM	2206	CZ3	TRP	274	-8 570	41.630	12.309	1 00	12.76
ATOM	2207	CH2	TRP	274	-8 591	40 765	13 403	1.00	12.58
ATOM	2208	C	TRP	274	-5 114	40 123	9 043	1.00	7.32
ATOM	2209	O	TRP	274	-6.156	40.621	8.598	1.00	8.37
ATOM	2210	N	VAL	275	-4.963	38 854	9.345	1 00	7 40
ATOM	2211	CA	VAL	275	-6 042	37 883	9.221	1 00	7 99
ATOM	2212	CB	VAL	275	-5.913	37.057	7.931	1.00	11.04
ATOM	2213	CG1	VAL	275	-7.152	36.169	7.828	1.00	13 41
ATOM	2214	CG2	VAL	275	-5.765	37.904	6 702	1.00	15.17
ATOM	2215	C	VAL	275	-5.933	37 000	10 457	1 00	7.32
ATOM	2216	O	VAL	275	-4.818	36.547	10 759	1 00	8 66
ATOM	2217	N	ASN	276	-7.013	36.774	11.175	1 00	7 50
ATOM	2218	CA	ASN	276	-6 930	35.898	12.365	1.00	8 58
ATOM	2219	CB	ASN	276	-7 921	36.377	13.414	1.00	9.69
ATOM	2220	CG	ASN	276	-7.600	35 733	14 757	1.00	10.43
ATOM	2221	OD1	ASN	276	-6.631	34.956	14.885	1.00	9.69
ATOM	2222	ND2	ASN	276	-8 414	35.995	15.765	1.00	12.06
ATOM	2223	C	ASN	276	-7.172	34.443	11.976	1.00	8.56
ATOM	2224	O	ASN	276	-8.281	33.914	12.021	1.00	9.02
ATOM	2225	N	ALA	277	-6.107	33.815	11.504	1 00	8.26
ATOM	2226	CA	ALA	277	-6.107	32.466	10.982	1 00	8.04
ATOM	2227	CB	ALA	277	-6.438	32.469	9.514	1.00	9.72
ATOM	2228	C	ALA	277	-4 711	31.860	11.136	1.00	7.91
ATOM	2229	O	ALA	277	-3 705	32 537	10.998	1.00	8.82
ATOM	2230	N	GLU	278	-4.674	30 592	11.445	1 00	7.51
ATOM	2231	CA	GLU	278	-3.460	29 801	11.557	1 00	7.98
ATOM	2232	CB	GLU	278	-3.727	28 504	12.302	1.00	10.38
ATOM	2233	CG	GLU	278	-2 539	27 650	12.655	1 00	11.75
ATOM	2234	CD	GLU	278	-1.613	28 347	13.638	1 00	10.88
ATOM	2235	OE1	GLU	278	-0.419	28 424	13.314	1.00	12.63
ATOM	2236	OE2	GLU	278	-2.074	28 833	14.680	1 00	10.57
ATOM	2237	C	GLU	278	-3.034	29.524	10.111	1 00	8.98
ATOM	2238	O	GLU	278	-3.719	28.836	9.346	1 00	12.15
ATOM	2239	N	ARG	279	-1.864	30.037	9.738	1.00	8.14
ATOM	2240	CA	ARG	279	-1.410	29.901	8.373	1.00	8.39
ATOM	2241	CB	ARG	279	-2.095	30 906	7.472	1.00	10.37
ATOM	2242	CG	ARG	279	-1.659	32.310	7 818	1.00	10.01
ATOM	2243	CD	ARG	279	-2.541	33.367	7.101	1.00	9.63
ATOM	2244	NE	ARG	279	-2.026	34 712	7.405	1.00	9.29
ATOM	2245	CZ	ARG	279	-0.965	35 208	6.775	1.00	9.20
ATOM	2246	NH1	ARG	279	-0.368	34 596	5.774	1.00	9.24
ATOM	2247	NH2	ARG	279	-0.490	36 396	7.129	1.00	9.29
ATOM	2248	C	ARG	279	0.095	29 920	8.275	1.00	7.13
ATOM	2249	O	ARG	279	0.821	30 149	9.252	1.00	8.10
ATOM	2250	N	GLN	280	0.593	29 601	7.095	1.00	7.21
ATOM	2251	CA	GLN	280	2.006	29 505	6.778	1.00	7.07
ATOM	2252	CB	GLN	280	2.318	28 088	6.255	1.00	8.87
ATOM	2253	CG	GLN	280	2.043	27 047	7.312	1.00	8.89
ATOM	2254	CD	GLN	280	2.188	25 645	6.771	1.00	8.58
ATOM	2255	OE1	GLN	280	2.067	25 442	5.571	1.00	11.01
ATOM	2256	NE2	GLN	280	2.533	24 689	7.591	1.00	8.97
ATOM	2257	C	GLN	280	2.389	30 454	5.653	1.00	6.21
ATOM	2258	O	GLN	280	1.634	30.606	4.671	1.00	7.53
ATOM	2259	N	SER	281	3.554	31.037	5.779	1.00	6.11

ATOM	2260	CA	SER	281	4.156	31.865	4.744	1.00	6.44
ATOM	2261	CB	SER	281	4.016	33.345	5.109	1.00	7.40
ATOM	2262	OG	SER	281	4.520	34.121	4.016	1.00	8.04
ATOM	2263	C	SER	281	5.617	31.443	4.606	1.00	6.56
ATOM	2264	O	SER	281	6.374	31.574	5.574	1.00	6.58
ATOM	2265	N	LEU	282	5.952	30.778	3.493	1.00	5.40
ATOM	2266	CA	LEU	282	7.243	30.105	3.352	1.00	6.03
ATOM	2267	CB	LEU	282	6.986	28.583	3.195	1.00	6.16
ATOM	2268	CG	LEU	282	8.982	27.942	4.203	1.00	7.21
ATOM	2269	CD1	LEU	282	8.851	26.441	3.942	1.00	8.79
ATOM	2270	CD2	LEU	282	6.340	28.186	5.661	1.00	8.29
ATOM	2271	C	LEU	282	8.025	30.642	2.173	1 00	5 52
ATOM	2272	O	LEU	282	8.055	30.039	1.071	1 00	5.66
ATOM	2273	N	PRO	283	8.632	31.801	2.318	1.00	5 55
ATOM	2274	CD	PRO	283	8 549	32.739	3.463	1.00	5 92
ATOM	2275	CA	PRO	283	9 437	32.349	1.222	1.00	5.72
ATOM	2276	CB	PRO	283	9 634	33.815	1.631	1 00	6.44
ATOM	2277	CG	PRO	283	9.624	33.748	3.131	1 00	6.28
ATOM	**2278**	**C**	**PRO**	**283**	**10.795**	**31.729**	**1.057**	**1 00**	**4.97**
ATOM	2279	O	PRO	283	11.445	31.322	2 006	1 00	5.92
ATOM	2280	N	PHE	284	11.262	31.720	-0 187	1.00	5 22
ATOM	2281	CA	PHE	284	12 642	31.498	-0 602	1.00	4 80
ATOM	2282	CB	PHE	284	12.785	30.323	-1.566	1.00	5 14
ATOM	2283	CG	PHE	284	14.184	29.960	-1 983	1 00	4.79
ATOM	2284	CD1	PHE	284	15 089	29.473	-1 057	1 00	5.39
ATOM	2285	CD2	PHE	284	14 591	30.026	-3 286	1 00	5.88
ATOM	2286	CE1	PHE	284	16.341	29.032	-2 451	1 00	5.76
ATOM	2287	CE2	PHE	284	15.828	29 633	-3 714	1.00	5.70
ATOM	2288	CZ	PHE	284	16.714	29 109	-2.787	1.00	5.57
ATOM	2289	C	PHE	284	13 119	32 795	-1 263	1 00	4.78
ATOM	2290	O	PHE	284	12 566	33 190	-2.308	1.00	5.98
ATOM	2291	N	PHE	285	14.114	33 446	-0 659	1.00	5.01
ATOM	2292	CA	PHE	285	14 656	34.687	-1 215	1.00	5.10
ATOM	2293	CB	PHE	285	15 058	35.637	-0 062	1 00	6.13
ATOM	2294	CG	PHE	285	13.858	36.096	0 747	1 00	6 38
ATOM	2295	CD1	PHE	285	13.665	35.656	2 044	1 00	6.54
ATOM	2296	CD2	PHE	285	12.909	36 933	0 195	1.00	6 45
ATOM	2297	CE1	PHE	285	12 534	36 014	2.765	1.00	7 21
ATOM	2298	CE2	PHE	285	11.782	37 303	0 891	1.00	7 45
ATOM	2299	CZ	PHE	285	11 610	36 853	2.177	1 00	7 71
ATOM	2300	C	PHE	285	15 812	34.333	-2 108	1 00	5 08
ATOM	2301	O	PHE	285	16 815	33 800	-1 608	1 00	6 02
ATOM	2302	N	VAL	286	15 658	34 588	-3 399	1 00	5 58
ATOM	2303	CA	VAL	286	16.696	34.255	-4 364	1.00	5 56
ATOM	2304	CB	VAL	286	16 104	34 056	-5 766	1 00	5.78
ATOM	2305	CG1	VAL	286	17.189	33 789	-6 814	1 00	7.42
ATOM	2306	CG2	VAL	286	15.065	32 922	-5.710	1.00	7.19
ATOM	2307	C	VAL	286	17 756	35 372	-4.347	1.00	5 98
ATOM	2308	O	VAL	286	17.569	36 453	-4 895	1 00	6 92
ATOM	2309	N	ASN	287	18.839	35 082	-3 642	1 00	5 82
ATOM	2310	CA	ASN	287	20.008	35 922	-3 466	1.00	6 12
ATOM	2311	CB	ASN	287	20.324	36.042	-1.971	1.00	6.40
ATOM	2312	CG	ASN	287	19.235	36 737	-1 183	1 00	6.67
ATOM	2313	OD1	ASN	287	18.623	37 682	-1 683	1.00	7.35
ATOM	2314	ND2	ASN	287	19.036	36.262	0 073	1 00	6.70
ATOM	2315	C	ASN	287	21.187	35.296	-4.216	1 00	5.72
ATOM	2316	O	ASN	287	21.271	34.072	-4.300	1.00	6.46
ATOM	2317	N	LEU	288	22.049	36 245	-4.781	1.00	6.71
ATOM	2318	CA	LEU	288	23.223	35 679	-5.499	1.00	6.46
ATOM	2319	CB	LEU	288	23.538	36 703	-6.595	1.00	7.57
ATOM	2320	CG	LEU	288	22.371	36 977	-7.570	1.00	8.20
ATOM	2321	CD1	LEU	288	22.819	37 998	-8.621	1.00	10.08
ATOM	2322	CD2	LEU	288	21.880	35 687	-9.189	1.00	8.32
ATOM	2323	C	LEU	288	24.381	35 444	-4.525	1.00	7.33
ATOM	2324	O	LEU	288	24.140	35.277	-3.317	1.00	8.59
ATOM	2325	N	GLY	289	25.607	35.358	-5.037	1.00	7.93
ATOM	2326	CA	GLY	289	26.765	35 216	-4.155	1.00	7.86
ATOM	2327	C	GLY	289	27.242	36.571	-3.667	1.00	7.24
ATOM	2328	O	GLY	289	26.890	37.634	-4.186	1.00	8.44
ATOM	2329	N	TYR	290	28.075	36.559	-2.633	1.00	7.71
ATOM	2330	CA	TYR	290	28.503	37.789	-1.986	1.00	8.91
ATOM	2331	CB	TYR	290	29.407	37.453	-0.813	1.00	9.56
ATOM	2332	CG	TYR	290	29.638	38.614	0.135	1.00	9.12

ATOM	2333	CD1	TYR	290	28.720	38.961	1.118	1.00	10.55
ATOM	2334	CE1	TYR	290	28.949	40.041	1 966	1.00	12 13
ATOM	2335	CD2	TYR	290	30.792	39.367	0 036	1.00	12 09
ATOM	2336	CE2	TYR	290	31.035	40.426	0.887	1 00	13.43
ATOM	2337	CZ	TYR	290	30.129	40.766	1 861	1 00	13 85
ATOM	2338	OH	TYR	290	30.407	41.847	2.679	1 00	16 61
ATOM	2339	C	TYR	290	29.196	38 783	-2 903	1 00	8 98
ATOM	2340	O	TYR	290	28.979	39 980	-2 814	1 00	9 66
ATOM	2341	N	ASP	291	30.009	38.246	-3 816	1.00	9 63
ATOM	2342	CA	ASP	291	30.738	39.081	-4.766	1.00	11.13
ATOM	2343	CB	ASP	291	32.143	38.545	-4.920	1 00	14 78
ATOM	2344	CG	ASP	291	33.015	38 830	-3.715	1 00	19 43
ATOM	2345	OD1	ASP	291	34.005	38.109	-3.515	1 00	30.38
ATOM	2346	OD2	ASP	291	32.776	39 787	-2 963	1 00	21.52
ATOM	2347	C	ASP	291	30.075	39 198	-6.123	1.00	10.76
ATOM	2348	O	ASP	291	30.676	39 770	-7 035	1.00	14.21
ATOM	2349	N	SER	292	28.867	38 636	-6.294	1.00	10 05
ATOM	2350	CA	SER	292	28.226	38.714	-7.606	1 00	9 39
ATOM	2351	CB	SER	292	26.908	37.921	-7.562	1.00	9.60
ATOM	2352	OG	SER	292	27.117	36.538	-7.241	1.00	10.02
ATOM	2353	C	SER	292	27.915	40.181	-7 922	1.00	9 65
ATOM	2354	O	SER	292	27.303	40 934	-7.170	1.00	10 11
ATOM	2355	N	VAL	293	28.284	40.587	-9.123	1 00	11 44
ATOM	2356	CA	VAL	293	27.948	41.879	-9.675	1.00	12.30
ATOM	2357	CB	VAL	293	29.177	42 809	-9 749	1 00	14 95
ATOM	2358	CG1	VAL	293	28.691	44.199	-10.166	1.00	20.38
ATOM	2359	CG2	VAL	293	29.947	42 902	-8 464	1 00	18.62
ATOM	2360	C	VAL	293	27.402	41.683	-11.091	1.00	13 15
ATOM	2361	O	VAL	293	27.976	41.020	-11.971	1 00	17.31
ATOM	2362	N	ILE	294	26.232	42.246	-11.309	1.00	13.36
ATOM	2363	CA	ILE	294	25.669	42.289	-12.650	1.00	16.26
ATOM	2364	CB	ILE	294	24.283	41 645	-12.648	1 00	18.21
ATOM	2365	CG2	ILE	294	23.540	41.879	-13.941	1 00	22.79
ATOM	2366	CG1	ILE	294	24.529	40.135	-12.350	1 00	19.50
ATOM	2367	CD1	ILE	294	23.255	39.371	-12.397	1 00	21.00
ATOM	2368	C	ILE	294	25.616	43.756	-13.059	1.00	14.95
ATOM	2369	O	ILE	294	25.193	44.619	-12.311	1.00	14.96
ATOM	2370	N	ASP	295	26.164	44.020	-14.235	1.00	15.39
ATOM	2371	CA	ASP	295	26.203	45.398	-14.709	1.00	16.58
ATOM	2372	CB	ASP	295	27.214	45.501	-15.857	1.00	23.82
ATOM	2373	CG	ASP	295	28.612	45.188	-15.298	1.00	30.17
ATOM	2374	OD1	ASP	295	29.304	44.457	-16.044	1.00	42.83
ATOM	2375	OD2	ASP	295	29.000	45.638	-14.184	1.00	32.91
ATOM	2376	C	ASP	295	24.803	45.841	-15.109	1 00	13.64
ATOM	2377	O	ASP	295	24.072	45.199	-15.856	1 00	14.07
ATOM	2378	N	PRO	296	24.390	46.969	-14.533	1 00	12.78
ATOM	2379	CD	PRO	296	25.049	47.684	-13 426	1 00	14.44
ATOM	2380	CA	PRO	296	23.029	47.467	-14 847	1 00	12.67
ATOM	2381	CB	PRO	296	22.877	48.659	-13.923	1.00	14.23
ATOM	2382	CG	PRO	296	23.840	48.351	-12 818	1.00	16.25
ATOM	2383	C	PRO	296	22.825	47.803	-16 319	1 00	12.63
ATOM	2384	O	PRO	296	23.750	48.221	-17.032	1.00	14.48
ATOM	2385	N	PHE	297	21.602	47.615	-16.800	1.00	11.48
ATOM	2386	CA	PHE	297	21.260	47.872	-18.195	1.00	11.96
ATOM	2387	CB	PHE	297	21.388	46 632	-19.046	1.00	12.04
ATOM	2388	CG	PHE	297	20.543	45.425	-18 690	1.00	12.30
ATOM	2389	CD1	PHE	297	19.390	45 126	-19 386	1.00	15.33
ATOM	2390	CD2	PHE	297	20.900	44.597	-17 664	1.00	12.58
ATOM	2391	CE1	PHE	297	18.648	44 005	-19.091	1.00	17.14
ATOM	2392	CE2	PHE	297	20.121	43 510	-17 311	1.00	14.52
ATOM	2393	CZ	PHE	297	18.969	43 235	-18.003	1.00	16.56
ATOM	2394	C	PHE	297	19.837	48.421	-18.246	1.00	13.07
ATOM	2395	O	PHE	297	19.162	48 472	-17.219	1.00	14.15
ATOM	2396	N	ASP	298	19.390	48 809	-19.429	1.00	16.06
ATOM	2397	CA	ASP	298	18.024	49 272	-19.601	1.00	15.45
ATOM	2398	CB	ASP	298	18.023	50 788	-19.547	1.00	17.44
ATOM	2399	CG	ASP	298	16.619	51 374	-19.488	1.00	17.86
ATOM	2400	OD1	ASP	298	15.634	50 717	-19.809	1.00	17.50
ATOM	2401	OD2	ASP	298	16.580	52.580	-19.143	1.00	20.86
ATOM	2402	C	ASP	298	17.436	48.753	-20.900	1.00	16.52
ATOM	2403	O	ASP	298	17.736	49.281	-21.973	1.00	17.05
ATOM	2404	N	PRO	299	16.541	47.776	-20.829	1.00	16.19
ATOM	2405	CD	PRO	299	16.199	47.050	-19.589	1.00	17.38

ATOM	2406	CA	PRO	299	15.887	47.212	-22.014	1.00	16.63
ATOM	2407	CB	PRO	299	15.397	45.853	-21 562	1.00	19.69
ATOM	2408	CG	PRO	299	15.676	45.745	-20 112	1.00	21.06
ATOM	2409	C	PRO	299	14.854	48.081	-22 726	1.00	17.45
ATOM	2410	O	PRO	299	14.213	47.662	-23 730	1.00	18.54
ATOM	2411	N	ARG	300	14.705	49.327	-22 232	1.00	16.34
ATOM	2412	CA	ARG	300	13 857	50.321	-22.881	1.00	18.12
ATOM	2413	CB	ARG	300	13 086	51.146	-21 833	1.00	19.33
ATOM	2414	CG	ARG	300	11 959	50.301	-21 242	1.00	21 93
ATOM	2415	CD	ARG	300	11.237	50.861	-20.020	1.00	25 26
ATOM	2416	NE	ARG	300	12 231	51.198	-19.046	1 00	30 85
ATOM	2417	CZ	ARG	300	12 429	51.701	-17 857	1 00	29.50
ATOM	2418	NH1	ARG	300	11.422	52.069	-17.096	1 00	32 95
ATOM	2419	NH2	ARG	300	13 671	51.781	-17.407	1 00	30 69
ATOM	2420	C	ARG	300	14 691	52 279	-23 726	1 00	17 96
ATOM	2421	O	ARG	300	14 138	52 081	-24.462	1 00	17 01
ATOM	2422	N	GLU	301	15 997	51.254	-23 552	1 00	17 71
ATOM	2423	CA	GLU	301	16.913	52.185	-24 206	1 00	19.38
ATOM	2424	C	GLU	301	17.619	51.524	-25.392	1 00	18 52
ATOM	2425	O	GLU	301	18.127	50 400	-25.261	1 00	17 52
ATOM	2426	CB	GLU	301	17.949	52 595	-23.157	1 00	23 66
ATOM	2427	CG	GLU	301	17.521	53.757	-22.322	1.00	27 35
ATOM	2428	CD	GLU	301	16 969	54.959	-23 059	1.00	32 53
ATOM	2429	OE1	GLU	301	17 705	55.499	-23 901	1.00	38 75
ATOM	2430	OE2	GLU	301	15.841	55.411	-22.764	1 00	38 29
ATOM	2431	N	PRO	302	17.667	52 160	-26 553	1 00	18 63
ATOM	2432	CD	PRO	302	17.042	53.464	-26 839	1.00	21 36
ATOM	2433	CA	PRO	302	18.277	51 571	-27.738	1.00	20 90
ATOM	2434	CB	PRO	302	18.222	52 693	-28 776	1.00	22.61
ATOM	2435	CG	PRO	302	17 001	53.446	-28.341	1 00	22.90
ATOM	2436	C	PRO	302	19.683	51.057	-27.579	1.00	21 62
ATOM	2437	O	PRO	302	19.874	49.926	-28 009	1 00	24.93
ATOM	2438	N	ASN	303	20 520	51.712	-26.771	1 00	21 61
ATOM	2439	CA	ASN	303	21 840	52 125	-26.582	1 00	22 90
ATOM	2440	CB	ASN	303	22 905	52 194	-26 448	1.00	26.88
ATOM	2441	CG	ASN	303	22 642	53 204	-25 353	1 00	27.57
ATOM	2442	OD1	ASN	303	21 822	52.996	-24.467	1 00	23.80
ATOM	2443	ND2	ASN	303	23 353	54 329	-25.453	1 00	29.21
ATOM	2444	C	ASN	303	21 931	50.221	-25.360	1.00	20 67
ATOM	2445	O	ASN	303	23 039	49 773	-25 049	1 00	23 78
ATOM	2446	N	GLY	304	20 847	49 989	-24 661	1 00	17 93
ATOM	2447	CA	GLY	304	20.793	49 190	-23 443	1.00	18.03
ATOM	2448	C	GLY	304	21 488	49 856	-22.276	1 00	17 52
ATOM	2449	O	GLY	304	21 576	49.239	-21.215	1 00	20 50
ATOM	2450	N	LYS	305	22 009	51 071	-22.342	1 00	18 09
ATOM	2451	CA	LYS	305	22 768	51 590	-21 208	1 00	20 79
ATOM	2452	C	LYS	305	21 921	52.252	-20 147	1.00	20 39
ATOM	2453	O	LYS	305	20 850	52.777	-20 392	1.00	21.26
ATOM	2454	CB	LYS	305	23 884	52 524	-21 675	1.00	24.72
ATOM	2455	CG	LYS	305	25.002	51 789	-22.421	1 00	30.61
ATOM	2456	CD	LYS	305	26.032	52 816	-22.869	1 00	36 33
ATOM	2457	CE	LYS	305	26.246	52.908	-24 360	1 00	39.54
ATOM	2458	NZ	LYS	305	27.649	52.574	-24.760	1.00	51 21
ATOM	2459	N	SER	306	22.461	52 202	-18.921	1.00	18 96
ATOM	2460	CA	SER	306	21.758	52 837	-17.816	1.00	19 30
ATOM	2461	CB	SER	306	21.210	51.732	-16.911	1.00	23.77
ATOM	2462	OG	SER	306	21.758	51 769	-15.640	1.00	26.38
ATOM	2463	C	SER	306	22.711	53.732	-17.050	1.00	16.95
ATOM	2464	O	SER	306	23.919	53.528	-16.996	1.00	20.29
ATOM	2465	N	ASP	307	22.159	54.728	-16.365	1.00	18.07
ATOM	2466	CA	ASP	307	22.902	55.647	-15.527	1.00	17.75
ATOM	2467	CB	ASP	307	22.343	57.066	-15.646	1.00	19.69
ATOM	2468	CG	ASP	307	22.554	57.644	-17.030	1.00	21.31
ATOM	2469	OD1	ASP	307	23.544	57.289	-17.717	1.00	25.76
ATOM	2470	OD2	ASP	307	21.697	58.413	-17.492	1.00	22.42
ATOM	2471	C	ASP	307	23.003	55.194	-14.083	1.00	17.12
ATOM	2472	O	ASP	307	23.267	55.998	-13.150	1.00	15.97
ATOM	2473	N	ARG	308	22.897	53.886	-13.877	1.00	18.84
ATOM	2474	CA	ARG	308	23.109	53.313	-12.542	1.00	17.51
ATOM	2475	CB	ARG	308	22.067	52.271	-12.242	1.00	16.86
ATOM	2476	CG	ARG	308	20.688	52.745	-11.848	1.00	15.69
ATOM	2477	CD	ARG	308	19.627	51.694	-11.982	1.00	18.04
ATOM	2478	NE	ARG	308	18.312	52.224	-11.687	1.00	17.41

ATOM	2479	CZ	ARG	308	17.733	52.219	-10.497	1.00	15.39
ATOM	2480	NH1	ARG	308	18.288	51.740	-9.404	1.00	14.58
ATOM	2481	NH2	ARG	308	16.517	52.713	-10.426	1 00	19 03
ATOM	2482	C	ARG	308	24.511	52 680	-12.443	1 00	18 59
ATOM	2483	O	ARG	308	25.055	52 218	-13.440	1.00	25 55
ATOM	2484	N	GLU	309	25.070	52 659	-11.241	1.00	18.16
ATOM	2485	CA	GLU	309	26.350	52.054	-10.946	1 00	19.38
ATOM	2486	CB	GLU	309	27 058	52.935	-9.907	1.00	21.98
ATOM	2487	CG	GLU	309	27.442	54.299	-10 501	1 00	25 52
ATOM	2488	CD	GLU	309	28.319	54.244	-11.731	1 00	30.05
ATOM	2489	OE1	GLU	309	29 244	53 401	-11 842	1 00	36.16
ATOM	2490	OE2	GLU	309	28 114	55 058	-12.663	1 00	37.66
ATOM	2491	C	GLU	309	26 233	50.607	-10.484	1.00	15 87
ATOM	2492	O	GLU	309	25.287	50 180	-9.826	1.00	14 89
ATOM	2493	N	PRO	310	27.164	49 735	-10.842	1.00	14 73
ATOM	2494	CD	PRO	310	28.275	50 012	-11 799	1.00	16.91
ATOM	2495	CA	PRO	310	27.152	48.348	-10.386	1.00	15.04
ATOM	2496	CB	PRO	310	28.419	47 733	-11.059	1.00	17.03
ATOM	2497	CG	PRO	310	28.700	48 625	-12.220	1.00	19.09
ATOM	2498	C	PRO	310	27.219	48 266	-8.874	1.00	13.88
ATOM	2499	O	PRO	310	27.841	49.068	-8.164	1.00	15.60
ATOM	2500	N	LEU	311	26.474	47.318	-8.360	1.00	12.14
ATOM	2501	CA	LEU	311	26.338	47 085	-6 922	1.00	11.25
ATOM	2502	CB	LEU	311	24.878	47.460	-6.615	1.00	13.56
ATOM	2503	CG	LEU	311	24.457	47.333	-5.180	1.00	13.90
ATOM	2504	CD1	LEU	311	25.339	48.120	-4.233	1.00	20.42
ATOM	2505	CD2	LEU	311	22.986	47.700	-5 047	1.00	17.32
ATOM	2506	C	LEU	311	26.572	45.604	-6.622	1.00	10.64
ATOM	2507	O	LEU	311	25.915	44.759	-7.247	1.00	11.74
ATOM	2508	N	SER	312	27.494	45.257	-5 728	1.00	10.37
ATOM	2509	CA	SER	312	27.725	43.854	-5.407	1.00	11.32
ATOM	2510	CB	SER	312	29.040	43.653	-4.645	1.00	13.83
ATOM	2511	OG	SER	312	28.821	43.933	-3.284	1.00	20.95
ATOM	2512	C	SER	312	26.576	43.311	-4.593	1.00	9.82
ATOM	2513	O	SER	312	26.000	44.059	-3.793	1.00	11.18
ATOM	2514	N	TYR	313	26.260	42.025	-4.815	1.00	9.06
ATOM	2515	CA	TYR	313	25.095	41.471	-4.152	1.00	8.56
ATOM	2516	CB	TYR	313	24.722	40.082	-4.734	1.00	9.03
ATOM	2517	CG	TYR	313	23.265	39.812	-4.375	1.00	7.11
ATOM	2518	CD1	TYR	313	22 290	40.192	-5.276	1.00	8.14
ATOM	2519	CE1	TYR	313	20.951	40.004	-5.038	1.00	8.04
ATOM	2520	CD2	TYR	313	22.871	39.273	-3.179	1.00	6.33
ATOM	2521	CE2	TYR	313	21.525	39.151	-2.889	1.00	6 78
ATOM	2522	CZ	TYR	313	20.558	39.481	-3.810	1.00	6 87
ATOM	2523	OH	TYR	313	19.227	39.413	-3.570	1.00	7.92
ATOM	2524	C	TYR	313	25.247	41.465	-2.642	1.00	8 88
ATOM	2525	O	TYR	313	24.295	41.721	-1.876	1.00	8 66
ATOM	2526	N	GLY	314	26.436	41.154	-2.137	1.00	9.27
ATOM	2527	CA	GLY	314	26.636	41.130	-0.699	1.00	10.93
ATOM	2528	C	GLY	314	26.438	42.475	-0.028	1.00	11.24
ATOM	2529	O	GLY	314	25.837	42.532	1.044	1.00	11.92
ATOM	2530	N	ASP	315	26.927	43.543	-0.658	1.00	12.52
ATOM	2531	CA	ASP	315	26.682	44.876	-0.145	1.00	13.51
ATOM	2532	C	ASP	315	25.178	45.169	-0.126	1.00	11.36
ATOM	2533	O	ASP	315	24.643	45.674	0.871	1.00	12.03
ATOM	2534	CB	ASP	315	27 367	45.918	-1.023	1.00	18.60
ATOM	2535	CG	ASP	315	28.845	46.015	-0.671	1.00	23.51
ATOM	2536	OD1	ASP	315	29 308	45.275	0.214	1 00	34.09
ATOM	2537	OD2	ASP	315	29 448	46 876	-1.358	1 00	38.29
ATOM	2538	N	TYR	316	24 538	44 902	-1.265	1 00	10.83
ATOM	2539	CA	TYR	316	23 095	45 065	-1.383	1.00	9.46
ATOM	2540	CB	TYR	316	22 621	44 578	-2 740	1 00	9.26
ATOM	2541	CG	TYR	316	21.130	44 397	-2.840	1.00	8.60
ATOM	2542	CD1	TYR	316	20.273	45 477	-3 037	1.00	8.34
ATOM	2543	CE1	TYR	316	18.913	45 293	-3 143	1.00	7 74
ATOM	2544	CD2	TYR	316	20.585	43 119	-2.768	1.00	7 91
ATOM	2545	CE2	TYR	316	19.210	42 953	-2 847	1.00	7 88
ATOM	2546	CZ	TYR	316	18.381	44.028	-3 021	1.00	7 84
ATOM	2547	OH	TYR	316	17.021	43.799	-3 101	1.00	8.21
ATOM	2548	C	TYR	316	22.328	44.386	-0 260	1.00	8 23
ATOM	2549	O	TYR	316	21.435	44.940	0.393	1.00	8.68
ATOM	2550	N	LEU	317	22.637	43.104	-0 045	1.00	8.47
ATOM	2551	CA	LEU	317	21.902	42.282	0.915	1.00	8.58

ATOM	2552	CB	LEU	317	22.285	40.787	8.743	1.00	8.79
ATOM	2553	CG	LEU	317	21.561	39.779	1.629	1 00	8.20
ATOM	2554	CD1	LEU	317	20.073	39.788	1.272	1 00	9.81
ATOM	2555	CD2	LEU	317	22.141	38.375	1 492	1 00	10.08
ATOM	2556	C	LEU	317	22.107	42.735	2 352	1 00	8.90
ATOM	2557	O	LEU	317	21.144	42.841	3 087	1 00	9.53
ATOM	2558	N	GLN	318	23.362	42.918	2 770	1 00	10.62
ATOM	2559	CA	GLN	318	23.625	43.262	4 185	1 00	12.66
ATOM	2560	CB	GLN	318	25 124	43.337	4 464	1.00	14.04
ATOM	2561	CG	GLN	318	25 445	43.620	5.905	1 00	19.74
ATOM	2562	CD	GLN	318	26 927	43.890	6.154	1 00	23.96
ATOM	2563	OE1	GLN	318	27 714	44.211	5 249	1 00	35.18
ATOM	2564	NE2	GLN	318	27.322	43.856	7 426	1.00	29 80
ATOM	2565	C	GLN	318	22 915	44.561	4 553	1 00	12 86
ATOM	2566	O	GLN	318	22.198	44.673	5.560	1.00	15 11
ATOM	2567	N	ASN	319	23 013	45.524	3.641	1 00	12 55
ATOM	2568	CA	ASN	319	22 346	46.806	3.917	1 00	14 03
ATOM	**2569**	**CB**	**ASN**	**319**	**23.012**	**47.860**	**3.043**	**1.00**	**20.38**
ATOM	2570	CG	ASN	319	24.469	48.100	3.472	1 00	27 04
ATOM	2571	OD1	ASN	319	24.837	48 041	4.669	1 00	36.52
ATOM	2572	ND2	ASN	319	25.310	48 297	2 465	1.00	38 86
ATOM	2573	C	ASN	319	20 844	46.703	3 764	1 00	11.80
ATOM	2574	O	ASN	319	20 143	47.296	4 593	1.00	11.96
ATOM	2575	N	GLY	320	20 312	45.946	2 806	1 00	9 58
ATOM	2576	CA	GLY	320	18 902	45 829	2.624	1 00	9 89
ATOM	2577	C	GLY	320	18 179	45.194	3 797	1.00	9 39
ATOM	2578	O	GLY	320	17.091	45 598	4 167	1.00	10.40
ATOM	2579	N	LEU	321	18.797	44 151	4 363	1 00	9 14
ATOM	2580	CA	LEU	321	18.153	43 464	5 485	1 00	9.96
ATOM	2581	CB	LEU	321	18 857	42 133	5 768	1.00	10 64
ATOM	2582	CG	LEU	321	18 723	41.078	4 638	1.00	10.47
ATOM	2583	CD1	LEU	321	19 399	39 826	5 109	1.00	15.39
ATOM	2584	CD2	LEU	321	17 262	40.824	4.233	1.00	12.12
ATOM	2585	C	LEU	321	18.108	44.339	6.710	1.00	10.07
ATOM	2586	O	LEU	321	17 089	44.340	7.437	1 00	10.21
ATOM	2587	N	VAL	322	19.176	45 095	6.956	1 00	10.17
ATOM	2588	CA	VAL	322	19.146	46 035	8 069	1 00	11.92
ATOM	2589	CB	VAL	322	20.532	46 687	8 252	1.00	14.76
ATOM	2590	CG1	VAL	322	20 397	47.770	9 346	1 00	20.10
ATOM	2591	CG2	VAL	322	21 537	45 651	8 753	1 00	21.00
ATOM	2592	C	VAL	322	18 095	47 100	7 854	1 00	10.68
ATOM	2593	O	VAL	322	17 346	47 521	8 741	1 00	12.21
ATOM	2594	N	SER	323	18 014	47.617	6 634	1.00	11.81
ATOM	2595	CA	SER	323	17.069	48.683	6 345	1 00	11.28
ATOM	2596	CB	SER	323	17 295	49.233	4 922	1 00	14 31
ATOM	2597	OG	SER	323	18 592	49.829	4 835	1.00	19 95
ATOM	2598	C	SER	323	15 625	48 220	6.522	1 00	11.18
ATOM	2599	O	SER	323	14.776	48 982	6 976	1.00	12.09
ATOM	2600	N	LEU	324	15 345	46 979	6 128	1 00	11 02
ATOM	2601	CA	LEU	324	13.986	46.458	6.212	1.00	9 92
ATOM	2602	CB	LEU	324	13 893	45.156	5 430	1.00	9 96
ATOM	2603	CG	LEU	324	12.522	44.506	5 348	1 00	9.98
ATOM	2604	CD1	LEU	324	11 448	45.393	4 776	1 00	11 33
ATOM	2605	CD2	LEU	324	12 658	43.214	4 571	1 00	11 39
ATOM	2606	C	LEU	324	13 576	46 326	7.679	1.00	10.28
ATOM	2607	O	LEU	324	12.422	46.540	8.070	1.00	10 32
ATOM	2608	N	ILE	325	14 532	45.886	8 497	1 00	10 22
ATOM	2609	CA	ILE	325	14 292	45 805	9 939	1.00	11.04
ATOM	2610	CB	ILE	325	15.451	45 120	10 669	1.00	10.87
ATOM	2611	CG2	ILE	325	15 398	45 298	12 164	1.00	13.93
ATOM	2612	CG1	ILE	325	15.454	43 605	10 363	1.00	12.46
ATOM	2613	CD1	ILE	325	16 785	42 944	10 725	1.00	15.56
ATOM	2614	C	ILE	325	14 040	47.192	10 522	1.00	10.74
ATOM	2615	O	ILE	325	13.122	47.404	11 341	1.00	11 60
ATOM	2616	N	ASN	326	14.819	48.181	10 151	1.00	10.99
ATOM	2617	CA	ASN	326	14.602	49.531	10 659	1.00	12.82
ATOM	2618	CB	ASN	326	15.732	50.459	10 168	1.00	14.29
ATOM	2619	CG	ASN	326	17.014	50.101	10.904	1.00	17.21
ATOM	2620	OD1	ASN	326	16.959	49.382	11.917	1.00	23.79
ATOM	2621	ND2	ASN	326	18.130	50.520	10.318	1.00	22.06
ATOM	2622	C	ASN	326	13.265	50.066	10.203	1.00	12.41
ATOM	2623	O	ASN	326	12.620	50.749	10.996	1.00	14.07
ATOM	2624	N	LYS	327	12.840	49.790	8.973	1.00	11.71

ATOM	2625	CA	LYS	327	11.586	50.307	8.468	1.00	12.41
ATOM	2626	CB	LYS	327	11.543	50.205	6 918	1.00	13.45
ATOM	2627	CG	LYS	327	10.362	50.865	6.259	1.00	18.26
ATOM	2628	CD	LYS	327	9 847	50.144	5.014	1.00	21 08
ATOM	2629	CE	LYS	327	8 605	50.768	4.423	1.00	21.51
ATOM	2630	NZ	LYS	327	7.335	50.650	5.211	1.00	17.68
ATOM	2631	C	LYS	327	10.349	49.653	9 067	1.00	11.15
ATOM	2632	O	LYS	327	9 389	50.327	9.506	1.00	12.52
ATOM	2633	N	ASN	328	10.358	48.303	8.990	1.00	10 58
ATOM	2634	CA	ASN	328	9.160	47.510	9.286	1.00	11.33
ATOM	2635	CB	ASN	328	8.762	46.614	8.084	1.00	14 02
ATOM	2636	CG	ASN	328	8.096	47.438	7.002	1.00	14.11
ATOM	2637	OD1	ASN	328	7 997	48.681	7.112	1.00	16.02
ATOM	2638	ND2	ASN	328	7.525	46.796	5.995	1.00	11 03
ATOM	2639	C	ASN	328	9.224	46 671	10.551	1.00	11.26
ATOM	2640	O	ASN	328	8.226	45.994	10.873	1.00	13.57
ATOM	2641	N	GLY	329	10.341	46.732	11.270	1 00	12.34
ATOM	2642	CA	GLY	329	10.445	46.076	12.554	1.00	12.29
ATOM	2643	C	GLY	329	11.146	44.739	12.523	1.00	11.30
ATOM	2644	O	GLY	329	11.221	44.056	11.517	1.00	11.94
ATOM	2645	N	GLN	330	11 716	44.359	13.668	1 00	11.96
ATOM	2646	CA	GLN	330	12 364	43.036	13.787	1 00	10.55
ATOM	2647	CB	GLN	330	13.193	42.950	15.072	1.00	11.32
ATOM	2648	CG	GLN	330	13.686	41.560	15.352	1.00	11.79
ATOM	2649	CD	GLN	330	14.755	41.131	14.371	1 00	10.04
ATOM	2650	OE1	GLN	330	15 804	41.744	14.168	1.00	13.20
ATOM	2651	NE2	GLN	330	14.469	40.024	13.733	1.00	11.43
ATOM	2652	C	GLN	330	11.291	41.961	13.747	1.00	10 94
ATOM	2653	O	GLN	330	10.401	41.952	14.592	1 00	12.29
ATOM	2654	N	THR	331	11.377	41.063	12.784	1.00	9.93
ATOM	2655	CA	THR	331	10.438	39.956	12.692	1 00	10.56
ATOM	2656	CB	THR	331	10.367	39.375	11.277	1.00	13.12
ATOM	2657	OG1	THR	331	11.627	38.829	10.872	1.00	14 79
ATOM	2658	CG2	THR	331	9.945	40.455	10.274	1 00	18.32
ATOM	2659	C	THR	331	10.801	38.843	13.669	1 00	9.68
ATOM	2660	O	THR	331	9.996	37.874	13.694	1 00	10 45
ATOM	2661	OT	THR	331	11.803	38.971	14.419	1.00	9 25
ATOM	2662	OW	WAT	333	9.679	28.766	-0.715	1 00	6.49
ATOM	2663	OW	WAT	334	19.171	27.783	10.936	1.00	7.24
ATOM	2664	OW	WAT	335	9.260	43.735	-4.195	1 00	8.08
ATOM	2665	OW	WAT	336	22.532	31.208	2.029	1.00	6 26
ATOM	2666	OW	WAT	337	28.595	34.041	- 1.151	1 00	7 97
ATOM	2667	OW	WAT	338	24.607	26.075	6 861	1.00	8 47
ATOM	2668	OW	WAT	339	-2.784	36.461	-0.561	1.00	8.55
ATOM	2669	OW	WAT	340	22.156	23.031	7 059	1.00	7 69
ATOM	2670	OW	WAT	341	14.777	39.110	1 828	1 00	8 58
ATOM	2671	OW	WAT	342	12.607	41.059	1 589	1 00	9 25
ATOM	2672	OW	WAT	343	-1.547	35.753	12.742	1.00	9 09
ATOM	2673	OW	WAT	344	15.859	16.926	12 366	1.00	8 72
ATOM	2674	OW	WAT	345	17.270	37.486	2.078	1.00	8 11
ATOM	2675	OW	WAT	346	3.657	33.965	-24 602	1.00	10.08
ATOM	2676	OW	WAT	347	25 532	21.232	-3 227	1.00	9.87
ATOM	2677	OW	WAT	348	-2.697	35.006	10.127	1.00	9.24
ATOM	2678	OW	WAT	349	-1 983	38.149	8 911	1.00	9.83
ATOM	2679	OW	WAT	350	2.708	25.709	10 377	1.00	10.06
ATOM	2680	OW	WAT	351	1.466	29.802	-2 581	1.00	10.39
ATOM	2681	OW	WAT	352	1.694	36.486	5 140	1.00	10.21
ATOM	2682	OW	WAT	353	14.787	40.054	-27 891	1.00	11.32
ATOM	2683	OW	WAT	354	7.944	41.566	-10.080	1.00	11.49
ATOM	2684	OW	WAT	355	10.898	19.364	-0 933	1.00	11.45
ATOM	2685	OW	WAT	356	11.246	44.075	8.852	1.00	10.27
ATOM	2686	OW	WAT	357	19.835	30.921	-23 876	1.00	12.14
ATOM	2687	OW	WAT	358	27.717	21.786	-4.790	1.00	10.92
ATOM	2688	OW	WAT	359	25.375	32.089	-5.869	1.00	11.81
ATOM	2689	OW	WAT	360	7.719	32.045	19 976	1.00	10.99
ATOM	2690	OW	WAT	361	12.903	41.900	8.252	1.00	10.19
ATOM	2691	OW	WAT	362	15.465	41.811	7.221	1.00	10.84
ATOM	2692	OW	WAT	363	12.347	17.857	1.029	1.00	12.37
ATOM	2693	OW	WAT	364	16.302	36.649	-24.739	1.00	10.86
ATOM	2694	OW	WAT	365	10.865	30.651	24.027	1.00	12.28
ATOM	2695	OW	WAT	366	19.416	33.418	-15.771	1.00	10.14
ATOM	2696	OW	WAT	367	0.655	27.761	10.957	1.00	11.04
ATOM	2697	OW	WAT	368	6.259	36.234	-3.794	1.00	11.14

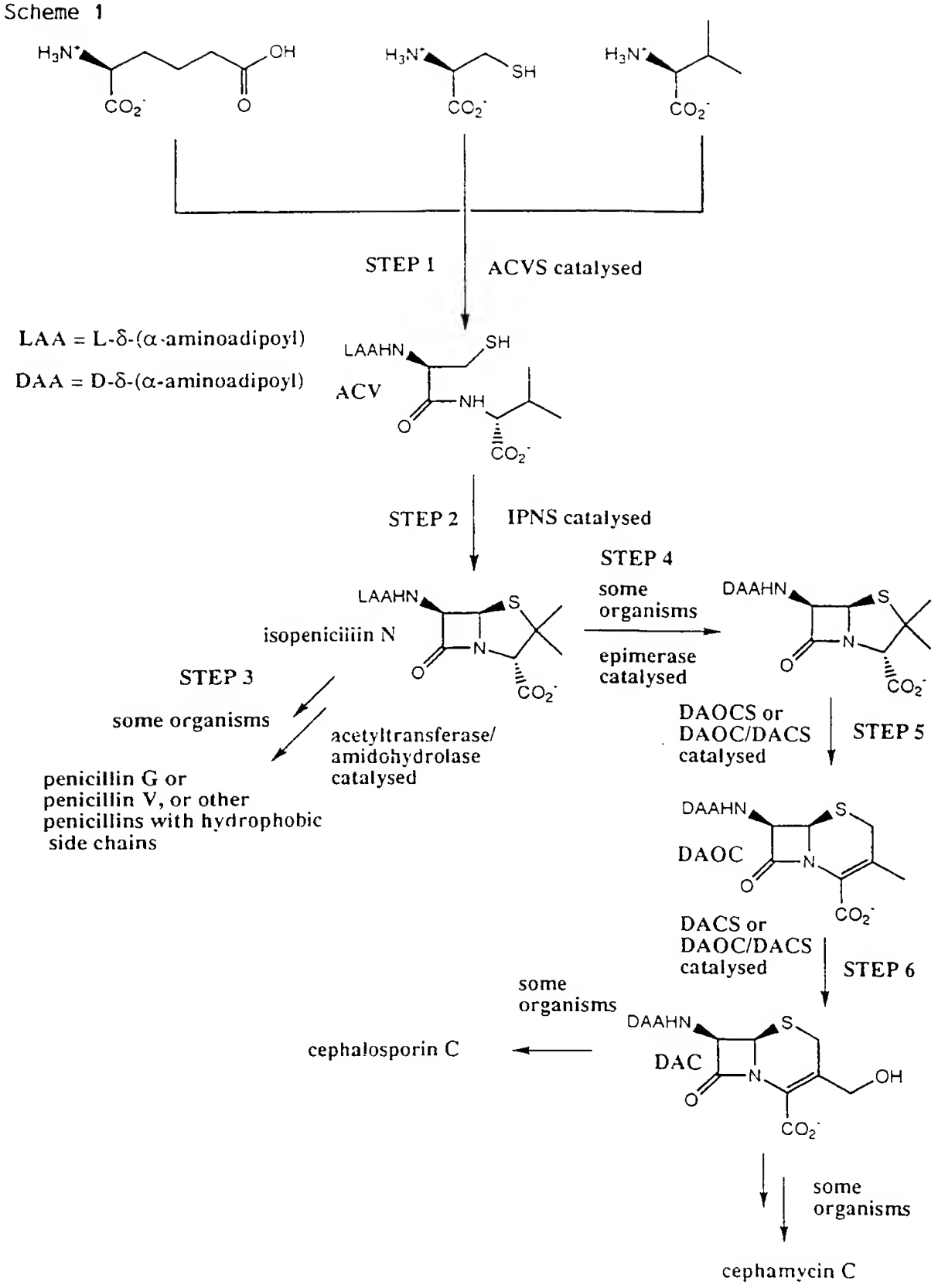
ATOM	2698	OW	WAT	369	16.675	14.973	9.695	1 00	11.88
ATOM	2699	OW	WAT	370	7.905	39.248	-11.909	1 00	10.25
ATOM	2700	OW	WAT	371	18.361	15.936	2.863	1 00	11.46
ATOM	2701	OW	WAT	372	21.892	19.503	1.831	1 00	13.37
ATOM	2702	OW	WAT	373	7.417	33.809	23.230	1.00	11.13
ATOM	2703	OW	WAT	374	9.301	18.255	-4.039	1.00	13.47
ATOM	2704	OW	WAT	375	5.788	38.293	-2.097	1 00	12.75
ATOM	2705	OW	WAT	376	21 318	28.084	18.230	1.00	13.18
ATOM	2706	OW	WAT	377	5 087	41.215	-22.821	1.00	13 37
ATOM	2707	OW	WAT	378	24.969	23.273	6.991	1.00	13 42
ATOM	2708	OW	WAT	379	11 227	49 320	-8.022	1 00	13 42
ATOM	2709	OW	WAT	380	-7 291	29.246	11.626	1 00	13 60
ATOM	2710	OW	WAT	381	5 640	46.235	9.550	1.00	13 85
ATOM	2711	OW	WAT	382	8 978	35.948	12.107	1 00	11 77
ATOM	2712	OW	WAT	383	6.906	29 370	22.628	1.00	15 24
ATOM	2713	OW	WAT	384	9.627	19.425	20.724	1 00	14 52
ATOM	2714	OW	WAT	385	16.459	39.497	8.314	1 00	14.01
ATOM	**2715**	**OW**	**WAT**	**386**	**24.545**	**45.847**	**-10.066**	**1.00**	**13.62**
ATOM	2716	OW	WAT	387	-0.150	40.151	23.142	1 00	15 04
ATOM	2717	OW	WAT	388	17.528	29 421	-23 847	1 00	12.67
ATOM	2718	OW	WAT	389	11.478	50 549	-25.585	1 00	14 89
ATOM	2719	OW	WAT	390	13 559	40.717	10.705	1.00	15 14
ATOM	2720	OW	WAT	391	8 290	18 854	-0.320	1.00	13.16
ATOM	2721	OW	WAT	392	18 743	43 137	-23 378	1.00	13.36
ATOM	2722	OW	WAT	393	-0 660	20.821	-4.126	1 00	14.45
ATOM	2723	OW	WAT	394	11 073	48.625	1.433	1 00	13.51
ATOM	2724	OW	WAT	395	21.541	28.028	-11.200	1 00	16 03
ATOM	2725	OW	WAT	396	-9 012	33 285	2 180	1.00	13 36
ATOM	2726	OW	WAT	397	-5 015	37 842	-7 595	1 00	14.72
ATOM	2727	OW	WAT	398	7 685	39 106	-0 476	1 00	13 04
ATOM	2728	OW	WAT	399	-2 609	52.730	2 926	1 00	15.18
ATOM	2729	OW	WAT	400	31 148	33 765	-2 024	1.00	15.90
ATOM	2730	OW	WAT	401	28 412	25.681	-6 948	1.00	14.37
ATOM	2731	OW	WAT	402	-7 837	33 960	-2 251	1.00	16 42
ATOM	2732	OW	WAT	403	27.733	30.817	11 858	1.00	16.15
ATOM	2733	OW	WAT	404	20 345	47 455	-0.111	1.00	15.84
ATOM	2734	OW	WAT	405	7 740	46.885	-13.836	1.00	15.47
ATOM	2735	OW	WAT	406	-6.948	43.028	7 219	1.00	13.61
ATOM	2736	OW	WAT	407	-1.255	31.160	-1 492	1 00	15.03
ATOM	2737	OW	WAT	408	-7.351	47.298	1 758	1 00	16 16
ATOM	2738	OW	WAT	409	0 600	50.511	3.412	1 00	16 57
ATOM	2739	OW	WAT	410	29 491	38 870	14.832	1 00	13 70
ATOM	2740	OW	WAT	411	19 032	29 394	25 238	1 00	13 82
ATOM	2741	OW	WAT	412	1 566	29.249	-3 495	1.00	12.61
ATOM	2742	OW	WAT	413	1.396	29.458	-19 005	1 00	17 83
ATOM	2743	OW	WAT	414	12 993	13.760	6 156	1.00	16 00
ATOM	2744	OW	WAT	415	-3.489	25 740	2 588	1 00	14 57
ATOM	2745	OW	WAT	416	20 400	16 258	4 749	1.00	15 12
ATOM	2746	OW	WAT	417	8.420	43 590	-11 863	1 00	15 17
ATOM	2747	OW	WAT	418	23 155	21 243	-4 704	1.00	15 01
ATOM	2748	OW	WAT	419	13.407	49.512	-6.246	1 00	18.08
ATOM	2749	OW	WAT	420	2 293	43.872	-19 188	1 00	15.75
ATOM	2750	OW	WAT	421	16 464	23.984	-12.729	1 00	16 55
ATOM	2751	OW	WAT	422	18 051	18 401	13 304	1 00	16 18
ATOM	2752	OW	WAT	423	2.749	32 610	17 294	1 00	16 03
ATOM	2753	OW	WAT	424	3.167	43.048	-21 870	1 00	16 60
ATOM	2754	OW	WAT	425	1.729	36 092	20.156	1 00	16 00
ATOM	2755	OW	WAT	426	24.912	30 437	18 039	1 00	18 10
ATOM	2756	OW	WAT	427	1.661	37.179	-17.778	1 00	16 68
ATOM	2757	OW	WAT	428	8.377	48 751	-17.456	1 00	17 96
ATOM	2758	OW	WAT	429	4.193	48 686	-6.577	1 00	16 18
ATOM	2759	OW	WAT	430	32.183	20 100	4.650	1.00	17 47
ATOM	2760	OW	WAT	431	10.701	20.889	-9.309	1 00	17 06
ATOM	2761	OW	WAT	432	1.230	36 624	-21.785	1 00	16 21
ATOM	2762	OW	WAT	433	23.224	53.219	-9.124	1 00	16 77
ATOM	2763	OW	WAT	434	7.454	14 204	-2.641	1 00	19 16
ATOM	2764	OW	WAT	435	-3.493	18.204	-1.008	1 00	16 26
ATOM	2765	OW	WAT	436	28.871	35.527	-9.186	1 00	16 44
ATOM	2766	OW	WAT	437	28.827	47.359	-4.440	1.00	20.15
ATOM	2767	OW	WAT	438	16.179	24.748	-15.541	1 00	18.41
ATOM	2768	OW	WAT	439	24.130	23.189	10.125	1.00	15.71
ATOM	2769	OW	WAT	440	9.413	18.353	13.315	1.00	22.18
ATOM	2770	OW	WAT	441	8.848	18.233	10.527	1.00	19.65

ATOM	2771	OW	WAT	442	26.464	32.534	18.217	1.00	16.18
ATOM	2772	OW	WAT	443	-7.877	38.342	4.061	1.00	17.91
ATOM	2773	OW	WAT	444	12.963	34.080	10.130	1.00	14.21
ATOM	2774	OW	WAT	445	5.117	27.600	16.871	1.00	17.53
ATOM	2775	OW	WAT	446	-9.839	37 847	2.096	1.00	20.90
ATOM	2776	OW	WAT	447	-1.745	32 409	3.793	1.00	20.56
ATOM	2777	OW	WAT	448	8.416	36.915	9.538	1.00	19.37
ATOM	2778	OW	WAT	449	13.442	46.906	0.805	1.00	15.63
ATOM	2779	OW	WAT	450	4.457	30 452	20.352	1.00	16.16
ATOM	2780	OW	WAT	451	8.792	16 265	-0.627	1.00	17.14
ATOM	2781	OW	WAT	452	-0.356	37.156	21.516	1.00	17.26
ATOM	2782	OW	WAT	453	11.477	23.152	-22.757	1.00	21.00
ATOM	2783	OW	WAT	454	21.490	29.901	24.676	1.00	18.12
ATOM	2784	OW	WAT	455	-9.438	38.109	10.367	1.00	20.23
ATOM	2785	OW	WAT	456	0.801	21 803	-6.497	1.00	16.76
ATOM	2786	OW	WAT	457	19.962	49 749	-14.695	1.00	19.53
ATOM	2787	OW	WAT	458	15.665	20 950	19.711	1.00	20.63
ATOM	2788	OW	WAT	459	22.253	42.588	7.507	1.00	18.83
ATOM	2789	OW	WAT	460	1.091	15.140	-0.991	1.00	17.62
ATOM	2790	OW	WAT	461	15.096	47.428	-1.171	1.00	18.28
ATOM	2791	OW	WAT	462	9.229	16.847	19.798	1.00	19.90
ATOM	2792	OW	WAT	463	23.458	31 087	22.465	1.00	20.21
ATOM	2793	OW	WAT	464	19.997	42.399	9.231	1.00	20.50
ATOM	2794	OW	WAT	465	-1.338	22.340	-1.994	1.00	18.86
ATOM	2795	OW	WAT	466	3.252	20.298	-7.395	1.00	20.44
ATOM	2796	OW	WAT	467	13.042	53.167	-27.095	1.00	19.91
ATOM	2797	OW	WAT	468	-10.643	37.955	25.133	1.00	20.65
ATOM	2798	OW	WAT	469	13.185	21.680	-8.488	1.00	20.52
ATOM	2799	OW	WAT	470	10.293	15.611	9.484	1.00	17.30
ATOM	2800	OW	WAT	471	18.301	39.511	-27.728	1.00	15.98
ATOM	2801	OW	WAT	472	30.497	24.989	-0.891	1.00	18.92
ATOM	2802	OW	WAT	473	34.106	27.545	11.353	1.00	20.62
ATOM	2803	OW	WAT	474	-1.263	34.235	-1.003	1.00	21.04
ATOM	2804	OW	WAT	475	30.740	34.281	8.033	1.00	22.42
ATOM	2805	OW	WAT	476	17.888	47.600	-24.851	1.00	19.76
ATOM	2806	OW	WAT	477	19.023	45.815	-22.920	1.00	19.37
ATOM	2807	OW	WAT	478	5.376	27.996	-23.488	1.00	23.73
ATOM	2808	OW	WAT	479	18.268	40.811	13.239	1.00	19.22
ATOM	2809	OW	WAT	480	-4.271	44.290	-11.498	1.00	18.91
ATOM	2810	OW	WAT	481	-10.443	35.240	1.254	1.00	19.73
ATOM	2811	OW	WAT	482	2.681	33.500	20.144	1.00	19.18
ATOM	2812	OW	WAT	483	19.770	15.947	12.144	1.00	20.32
ATOM	2813	OW	WAT	484	4.713	13.467	7.499	1.00	21.46
ATOM	2814	OW	WAT	485	-8.355	31.805	-0.398	1.00	23.32
ATOM	2815	OW	WAT	486	15.331	47.230	2.640	1.00	18.04
ATOM	2816	OW	WAT	487	25.206	36.975	8.919	1.00	23.97
ATOM	2817	OW	WAT	488	2.787	39 754	14.409	1.00	18.16
ATOM	2818	OW	WAT	489	2.364	46.924	-9.024	1.00	21.20
ATOM	2819	OW	WAT	490	18.912	42.320	-26.268	1.00	19.59
ATOM	2820	OW	WAT	491	9.332	14 150	-7 989	1.00	22.28
ATOM	2821	OW	WAT	492	3.716	51.522	-5.917	1.00	20.14
ATOM	2822	OW	WAT	493	30.485	19.369	6.691	1.00	22.71
ATOM	2823	OW	WAT	494	-8.748	45.801	7.529	1.00	21.63
ATOM	2824	OW	WAT	495	11.868	16.205	-2.683	1.00	21.66
ATOM	2825	OW	WAT	496	13.346	35.997	8.497	1.00	19.24
ATOM	2826	OW	WAT	497	0.972	40.899	-13.028	1.00	21 95
ATOM	2827	OW	WAT	498	4.183	53.535	-1.459	1.00	28.32
ATOM	2828	OW	WAT	499	30.346	39.016	-10.546	1.00	20.11
ATOM	2829	OW	WAT	500	16.129	24.513	-19.240	1.00	25.21
ATOM	2830	OW	WAT	501	10.923	41.632	17.779	1.00	28 12
ATOM	2831	OW	WAT	502	18.809	24.865	-19.164	1.00	22 89
ATOM	2832	OW	WAT	503	16.648	14.113	0.751	1.00	19 20
ATOM	2833	OW	WAT	504	19.213	39.701	8.979	1.00	20 79
ATOM	2834	OW	WAT	505	24.711	56.540	-10.148	1.00	20.81
ATOM	2835	OW	WAT	506	22.101	29.548	-23 677	1.00	22 77
ATOM	2836	OW	WAT	507	21 631	41.072	20 961	1.00	24.26
ATOM	2837	OW	WAT	508	-3 925	32.996	-15 355	1.00	25 98
ATOM	2838	OW	WAT	509	-3 683	27.982	6 567	1.00	23 91
ATOM	2839	OW	WAT	510	22 548	22 934	15 189	1.00	24.78
ATOM	2840	OW	WAT	511	3 233	21 643	-9.764	1.00	21 05
ATOM	2841	OW	WAT	512	33 443	23 225	2.328	1.00	24 54
ATOM	2842	OW	WAT	513	24 602	43 728	-18.078	1.00	25 43
ATOM	2843	OW	WAT	514	16.686	43 816	15.797	1.00	22 61

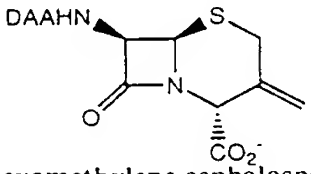
ATOM	2844	OW	WAT	515	10.964	18.976	-6.714	1.00	26.05
ATOM	2845	OW	WAT	516	0.840	16.582	-3.289	1.00	22.32
ATOM	2846	OW	WAT	517	-3.923	22.464	-1.744	1.00	29.01
ATOM	2847	OW	WAT	518	-0.997	25.906	9 408	1.00	27 67
ATOM	2848	OW	WAT	519	3.066	45.067	-23 581	1.00	21.23
ATOM	2849	OW	WAT	520	20 631	16.301	16 915	1.00	29 84
ATOM	2850	OW	WAT	521	3.683	28.042	-20.317	1.00	29 99
ATOM	2851	OW	WAT	522	-7 926	27.757	3.844	1.00	23.89
ATOM	2852	OW	WAT	523	1 150	23.857	-9.846	1.00	21 74
ATOM	2853	OW	WAT	524	13 889	16.199	-5.074	1.00	22.55
ATOM	2854	OW	WAT	525	-1 704	53.692	-2.952	1.00	32.09
ATOM	2855	OW	WAT	526	30 576	35 496	-4 718	1.00	26.56
ATOM	2856	OW	WAT	527	7 959	27 774	-32 333	1.00	22.85
ATOM	2857	OW	WAT	528	0 310	29 649	-17.650	1.00	26 17
ATOM	2858	OW	WAT	529	-0.573	40 681	-15.285	1.00	24 02
ATOM	2859	OW	WAT	530	-5 413	37.314	-11.579	1.00	26.13
ATOM	2860	OW	WAT	531	20.453	25 296	-22.221	1.00	26.01
ATOM	2861	OW	WAT	532	2.287	15.472	-5.046	1.00	27.90
ATOM	2862	OW	WAT	533	30.000	42.526	-1.756	1 00	25 99
ATOM	2863	OW	WAT	534	13.014	48.338	13.867	1.00	29 93
ATOM	2864	OW	WAT	535	19.089	59.470	-16.490	1.00	25 60
ATOM	2865	OW	WAT	536	23.246	37.608	-22.518	1.00	30.37
ATOM	2866	OW	WAT	537	18 012	23 775	-22 832	1.00	35 14
ATOM	2867	OW	WAT	538	32 942	31.103	-1 587	1.00	27 55
ATOM	2868	OW	WAT	539	24.244	39 395	8.376	1.00	26 84
ATOM	2869	OW	WAT	540	16 152	39 516	11.126	1.00	27.39
ATOM	2870	OW	WAT	541	-9 496	38.640	6.232	1.00	23.00
ATOM	2871	OW	WAT	542	11.570	53 681	-24.197	1.00	25 04
ATOM	2872	OW	WAT	543	5.652	39 623	9 901	1.00	24.86
ATOM	2873	OW	WAT	544	15.243	51.336	-7.590	1.00	31.58
ATOM	2874	OW	WAT	545	21.732	45.731	-22 796	1.00	25.40
ATOM	2875	OW	WAT	546	26.109	29.562	15.747	1.00	26.48
ATOM	2876	OW	WAT	547	5 300	48 774	10.712	1.00	22.97
ATOM	2877	OW	WAT	548	16 333	19.082	-6 041	1.00	31.87
ATOM	2878	OW	WAT	549	34.477	39.693	-0 433	1.00	24.27
ATOM	2879	OW	WAT	550	32.307	28.802	-2 454	1.00	28.07
ATOM	2880	OW	WAT	551	16.750	23.348	20.119	1.00	30.93
ATOM	2881	OW	WAT	552	19.254	45.692	25.110	1.00	30.02
ATOM	2882	OW	WAT	553	7.615	43 287	12.031	1.00	31.35
ATOM	2883	OW	WAT	554	21.139	41.273	15 275	1.00	24.54
ATOM	2884	OW	WAT	555	-9.531	43 159	1.000	1.00	28.18
ATOM	2885	OW	WAT	556	-4.562	35 560	22.961	1.00	25.96
ATOM	2886	OW	WAT	557	19.748	24.192	-10.428	1.00	29.93
ATOM	2887	OW	WAT	558	10.358	13 845	7.421	1.00	24.97
ATOM	2888	OW	WAT	559	33.144	26 300	-1.473	1.00	23.51
ATOM	2889	OW	WAT	560	0.711	42 085	-22.328	1.00	27.47
ATOM	2890	OW	WAT	561	19.258	55.289	-14.564	1.00	25.35
ATOM	2891	OW	WAT	562	13.683	49.398	-2.033	1.00	27.95
ATOM	2892	OW	WAT	563	21.974	39.944	7.537	1.00	24.21
ATOM	2893	OW	WAT	564	14.094	24.261	-29.685	1.00	30.81
ATOM	2894	OW	WAT	565	8.391	16.742	16.583	1.00	33.63
ATOM	2895	OW	WAT	566	34.902	40.206	3.922	1.00	34.09
ATOM	2896	OW	WAT	567	7.246	39.309	7.727	1.00	25.05
ATOM	2897	OW	WAT	568	1.772	52.043	-7.936	1.00	33.11
ATOM	2898	OW	WAT	569	-10 176	35.406	-1.420	1.00	28.71
ATOM	2899	OW	WAT	570	19 034	21.727	-6.972	1.00	31.14
ATOM	2900	OW	WAT	571	25.186	25.032	13.807	1.00	29.45
ATOM	2901	OW	WAT	572	-0.477	22.506	0.681	1.00	29.75
ATOM	2902	OW	WAT	573	7.554	13.615	9.613	1 00	25.51
ATOM	2903	OW	WAT	574	0.741	35.993	-6.797	1.00	28.22
ATOM	2904	OW	WAT	575	4.524	26.932	19.683	1 00	30.25
ATOM	2905	OW	WAT	576	24.217	31.560	29.964	1 00	30.98
ATOM	2906	OW	WAT	577	-9.886	38.987	-0.391	1 00	30.58
ATOM	2907	OW	WAT	578	18.264	48.710	-5.256	1 00	26.25
ATOM	2908	OW	WAT	579	7.094	48.558	-19.857	1 00	30.55
ATOM	2909	OW	WAT	580	-11.403	38.772	12.578	1.00	23.49
ATOM	2910	OW	WAT	581	0.236	53.067	3.666	1.00	32.85
ATOM	2911	OW	WAT	582	34.494	30.211	11.953	1.00	30.38
ATOM	2912	OW	WAT	583	-8.883	40.085	8.563	1.00	20.61
ATOM	2913	OW	WAT	584	19.648	16.274	-1 256	1.00	32.05
ATOM	2914	OW	WAT	585	0.789	53.240	6.163	1.00	28.48
ATOM	2915	OW	WAT	586	6.772	16.061	19.133	1.00	28.67
ATOM	2916	OW	WAT	587	17.572	48.350	-0.455	1.00	31.70

ATOM	2917	OW	WAT	588	19.914	42.743	12.082	1.00	29.47
ATOM	2918	OW	WAT	589	28.293	43 369	3.095	1.00	41.10
ATOM	2919	OW	WAT	590	4.140	16.905	-6.015	1.00	33.04
ATOM	2920	OW	WAT	591	-7.536	49.473	0.700	1.00	26.21
ATOM	2921	OW	WAT	592	16.545	11.527	7.703	1.00	35.77
ATOM	2922	OW	WAT	593	21.751	26.587	-18.455	1.00	36.98
ATOM	2923	OW	WAT	594	28.027	36.486	9.408	1.00	30.24
ATOM	2924	OW	WAT	595	-3.668	27 781	16.465	1.00	32.59
ATOM	2925	OW	WAT	596	6.641	50.716	9.132	1.00	30.57
ATOM	2926	OW	WAT	597	14.904	54.419	-12.497	1.00	35.34
ATOM	2927	OW	WAT	598	13.687	41.518	18.737	1.00	28.20
ATOM	2928	OW	WAT	599	15 809	10.449	13.628	1.00	27.51
ATOM	2929	OW	WAT	600	0.266	35.585	-19.094	1.00	32.22
ATOM	2930	OW	WAT	601	1.157	32.250	-2.186	1.00	31.93
ATOM	2931	OW	WAT	602	20.830	54.594	-22.978	1.00	38.78
ATOM	2932	OW	WAT	603	-6.482	24.335	0.209	1.00	27.40
ATOM	2933	OW	WAT	604	-0 221	24.757	-19.652	1.00	34.87
ATOM	2934	OW	WAT	605	4.475	41.359	13.507	1.00	38.95
ATOM	2935	OW	WAT	606	18.365	17 118	-5.002	1.00	35.63
ATOM	2936	OW	WAT	607	10.129	37.103	7.607	1.00	37.59
ATOM	2937	OW	WAT	608	32.483	26.313	-6.257	1.00	34.83
ATOM	2938	OW	WAT	609	1.173	18.896	13.815	1.00	38.79
ATOM	2939	OW	WAT	610	21.714	21.650	-7.187	1.00	30.79
ATOM	2940	OW	WAT	611	16.630	13.196	3.673	1.00	38.22
ATOM	2941	OW	WAT	612	3.332	18.798	15.551	1.00	30.36
ATOM	2942	OW	WAT	613	11.410	46.061	15.908	1.00	30.96
ATOM	2943	OW	WAT	614	1.890	53.075	0.396	1.00	35.43
ATOM	2944	OW	WAT	615	14.858	54.460	-19.563	1.00	36.48
ATOM	2945	OW	WAT	616	27.164	22.302	9.178	1.00	28.96
ATOM	2946	OW	WAT	617	25.844	30.643	13.373	1.00	37.70
ATOM	2947	OW	WAT	618	-11.773	30.992	19.536	1.00	35.27
ATOM	2948	OW	WAT	619	20.068	54.715	-26.556	1.00	30.61
ATOM	2949	OW	WAT	620	22.511	25.529	18.055	1.00	39.02
ATOM	2950	OW	WAT	621	4.762	24.578	19.147	1.00	29.70
ATOM	2951	OW	WAT	622	-5.809	31.212	-7.251	1.00	38.52
ATOM	2952	OW	WAT	623	2.302	46.734	-19.134	1.00	31.35
ATOM	2953	OW	WAT	624	-3.267	26.845	-9.657	1.00	26.55
ATOM	2954	OW	WAT	625	20.942	19.909	15.987	1.00	30.93
ATOM	2955	OW	WAT	626	14.335	19.417	27.897	1.00	41.36
ATOM	2956	OW	WAT	627	-8.960	44.991	2.623	1.00	32.33
ATOM	2957	OW	WAT	628	-2.896	18.495	3.945	1.00	33.15
ATOM	2958	OW	WAT	629	19.081	15.066	19.313	1.00	41.85
ATOM	2959	OW	WAT	630	26.583	40.965	-16.598	1.00	53.36
ATOM	2960	OW	WAT	631	9.201	30.845	-29.283	1.00	26.67
ATOM	2961	OW	WAT	632	29.771	29 232	13.030	1.00	37.22
ATOM	2962	OW	WAT	633	-9.063	44.258	5.485	1.00	30.64
ATOM	2963	OW	WAT	634	36.469	24.114	2.218	1.00	34.07
ATOM	2964	OW	WAT	635	1.658	28 923	20.644	1.00	39.44
ATOM	2965	OW	WAT	636	-8.637	37 196	-3.769	1.00	39.41
ATOM	2966	OW	WAT	637	9.491	43.672	18.552	1.00	34.67
ATOM	2967	OW	WAT	638	38.446	24.948	5.405	1.00	37.88
ATOM	2968	OW	WAT	639	16.362	21.306	-12.437	1.00	35.82
ATOM	2969	OW	WAT	640	11.407	51.004	-0.072	1.00	31.55
ATOM	2970	OW	WAT	641	38.229	24.335	8.085	1.00	39.89
ATOM	2971	OW	WAT	642	21.655	26.806	22.131	1.00	32.81
ATOM	2972	OW	WAT	643	16.387	22.635	23.545	1.00	35.28
ATOM	2973	OW	WAT	644	-12.122	42.861	-8.757	1.00	43.21
ATOM	2974	OW	WAT	645	-1.768	30.006	19.108	1.00	39.03
ATOM	2975	OW	WAT	646	31 231	36.441	-7.964	1.00	40.74
ATOM	2976	OW	WAT	647	-9.784	38.920	18.620	1.00	37.25
ATOM	2977	OW	WAT	648	-5.666	31.659	21 328	1.00	32.24
ATOM	2978	OW	WAT	649	-2 584	54.436	0.499	1 00	42.36
ATOM	2979	OW	WAT	650	9 314	15.276	13.185	1.00	41.13
ATOM	2980	OW	WAT	651	20.108	12.329	9.346	1 00	30.57
ATOM	2981	OW	WAT	652	28.719	20.042	8.674	1 00	30.27
ATOM	2982	OW	WAT	653	27.567	35.432	11.915	1.00	34.47
ATOM	2983	OW	WAT	654	20.822	18.155	14.214	1.00	29.75
ATOM	2984	OW	WAT	655	-1.395	25.107	7.194	1.00	42.08
END									

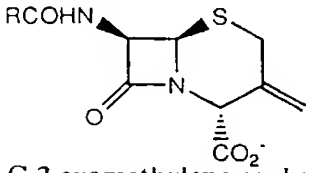
Scheme 1



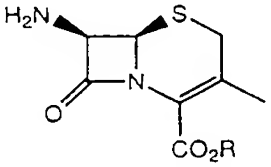
Scheme 2



exomethylene cephalosporin C

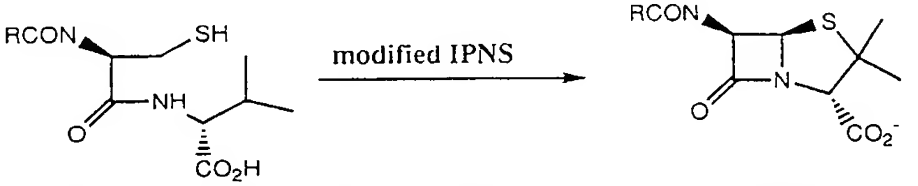


C-3 exomethylene cephams with hydrophobic side chains, e.g. R = $PhCH_2$, R = $PhOCH_2$, R = $HO_2C(CH_2)_4$



7-aminocephalosporins

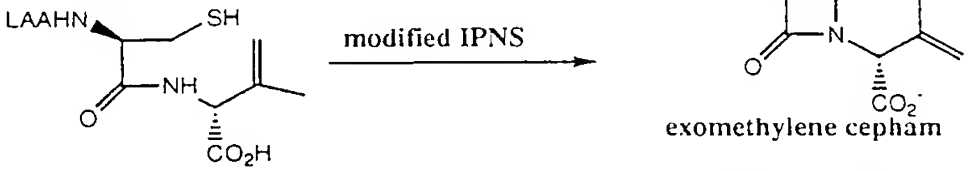
Scheme 5



where, R = alkyl or aryl or a combination of both, *e.g.* $PHCH_2$, $PhOCH_2$. The alkyl chain or aryl portion of R may also be substituted with acidic or basic groups, *e.g.* R = $HO_2C(CH_2)_4$, R = $H2N(CH_2)_4$. R may also be heterocyclic.

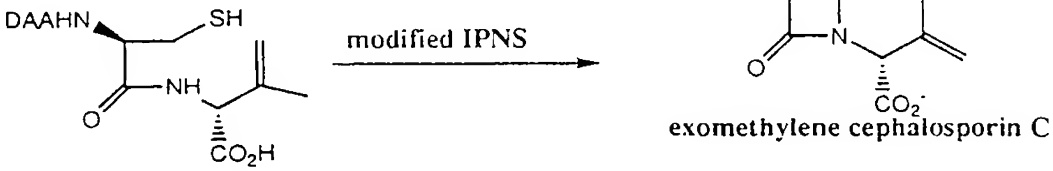
Scheme 6

example 1



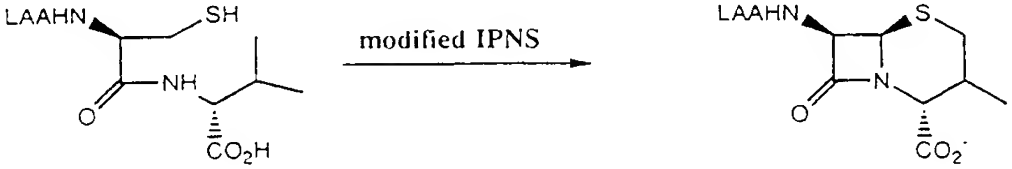
exomethylene cepham

example 2



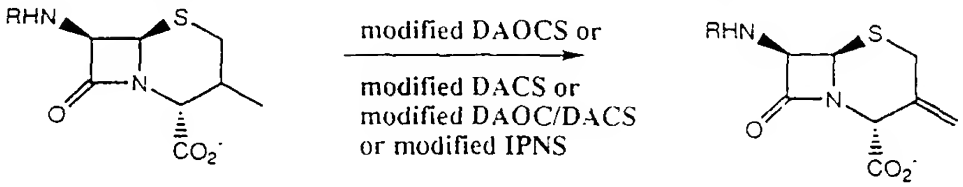
exomethylene cephalosporin C

example 3



Scheme 6 (cont.)

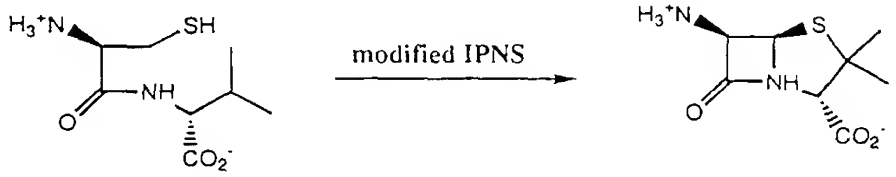
example 3 (cont.) The modified IPNS may be used in conjunction with another modified (or unmodified) enzyme activity, such as:



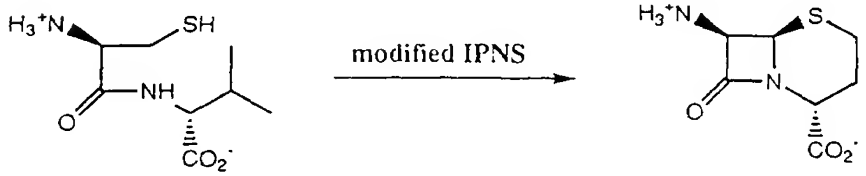
where R = LAA, DAA or other.

Scheme 7

example 1

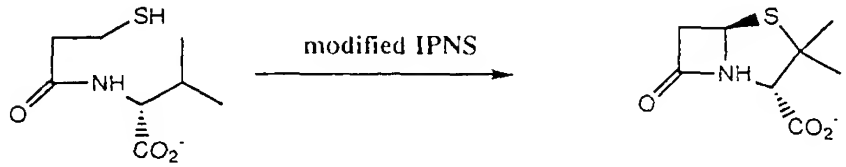


example 2

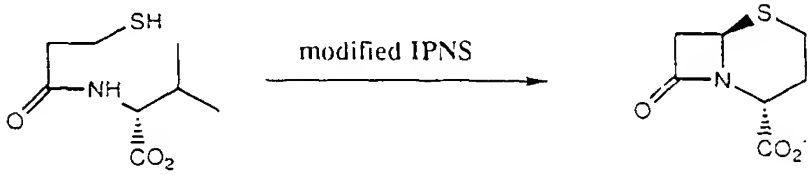


Scheme 8

example 1

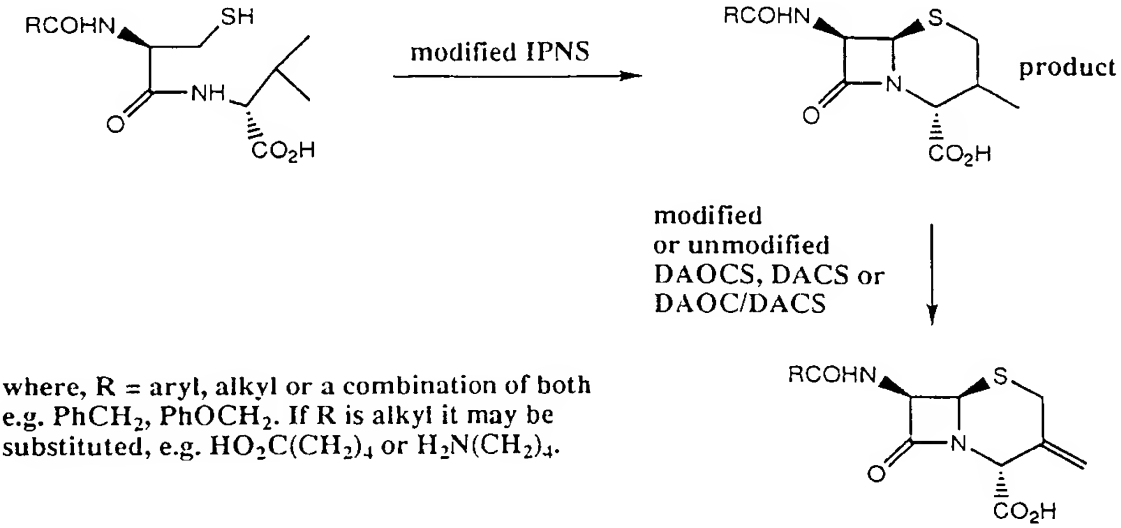


example 2



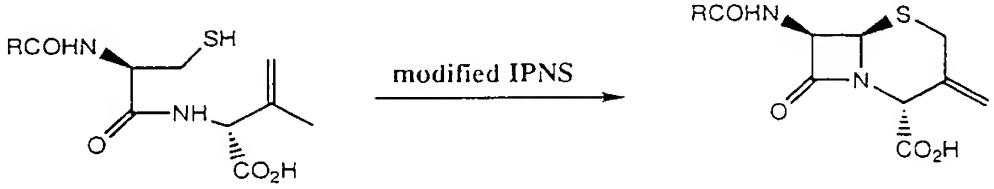
Scheme 9

example 1



where, R = aryl, alkyl or a combination of both e.g. $PhCH_2$, $PhOCH_2$. If R is alkyl it may be substituted, e.g. $HO_2C(CH_2)_4$ or $H_2N(CH_2)_4$.

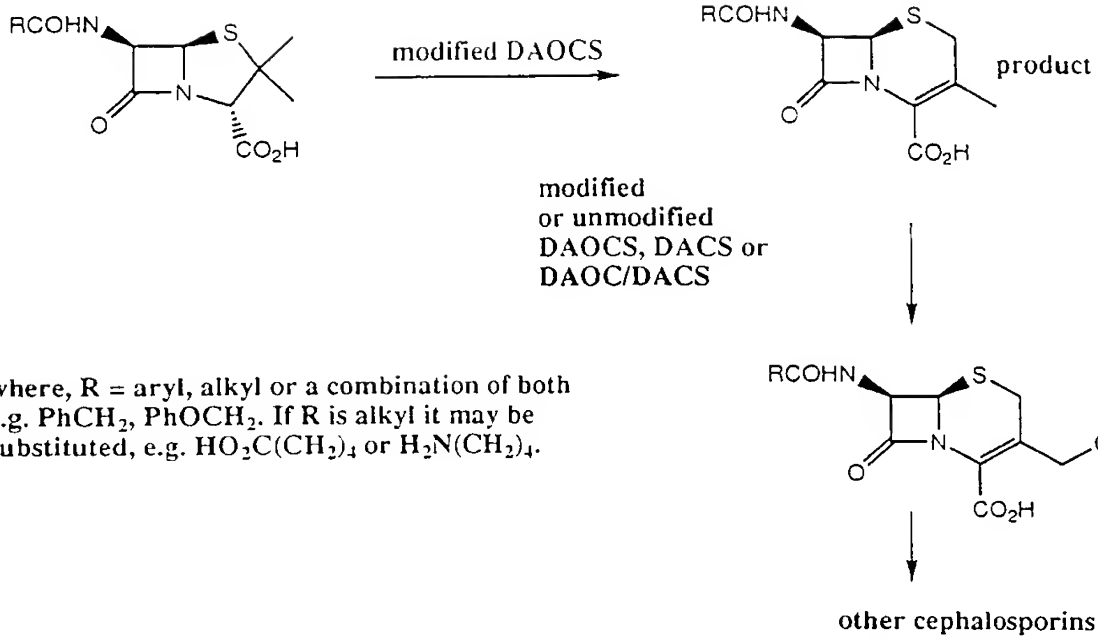
example 2



where, R = aryl, alkyl or a combination of both e.g. $PhCH_2$, $PhOCH_2$. If R is alkyl it may be substituted, e.g. $HO_2C(CH_2)_4$ or $H_2N(CH_2)_4$.
R = D-δ-(α-aminoadipoyl).

Scheme 10

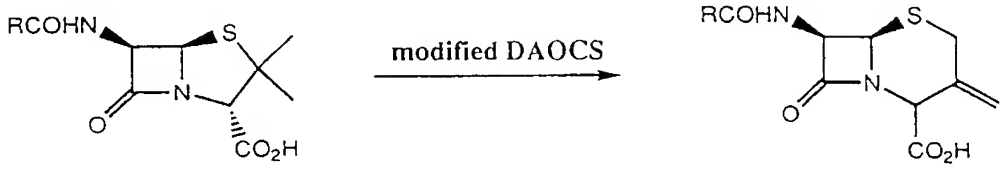
examples



where, R = aryl, alkyl or a combination of both e.g. $PhCH_2$, $PhOCH_2$. If R is alkyl it may be substituted, e.g. $HO_2C(CH_2)_4$ or $H_2N(CH_2)_4$.

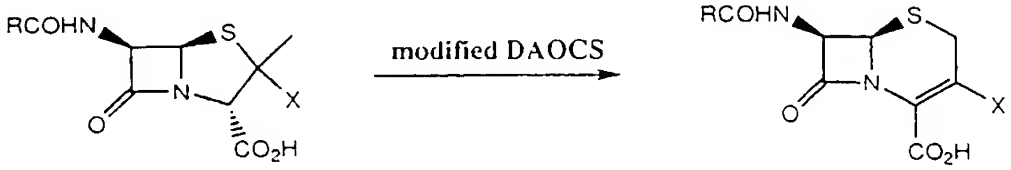
Scheme 11

example 1



where, R = D-δ-(α-aminoadipoyl), L-δ-(α-aminoadipoyl) $HO_2C(CH_2)_4$ or $H_2N(CH_2)_4$.

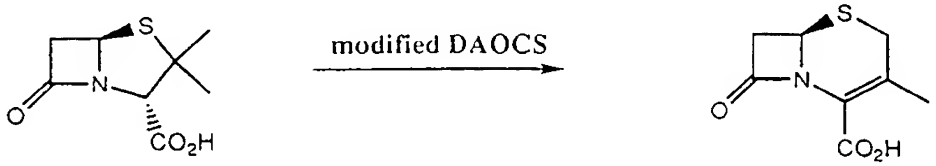
example 2



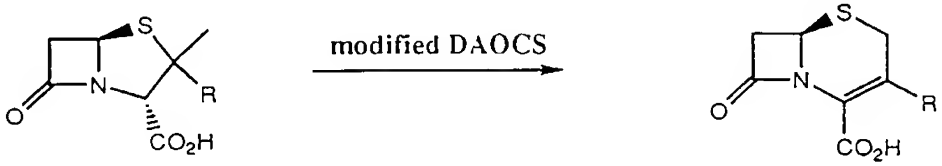
where, R = D-δ-(α-aminoadipoyl), D-δ-(α-aminoadipoyl) $HO_2C(CH_2)_4$ or $H_2N(CH_2)_4$, X = Cl, Br, I, OMe, SMe, or other substituent.

Scheme 13

example 1



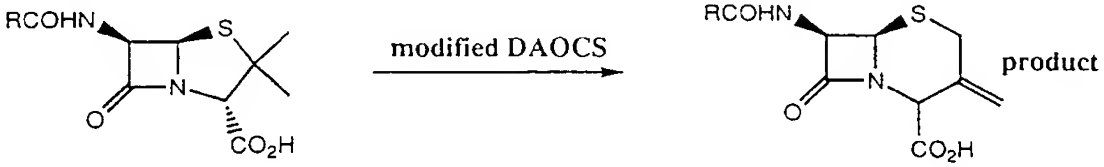
example 2



where R = Cl, Br, I, OMe or other substituent.

Scheme 14

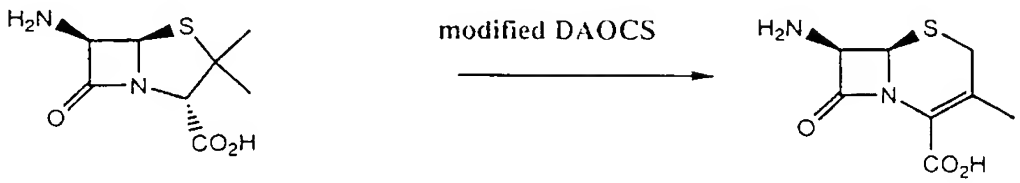
examples



where, R = aryl, alkyl or a combination of aryl and alkyl
e.g. $PhCH_2$, $PhOCH_2$.

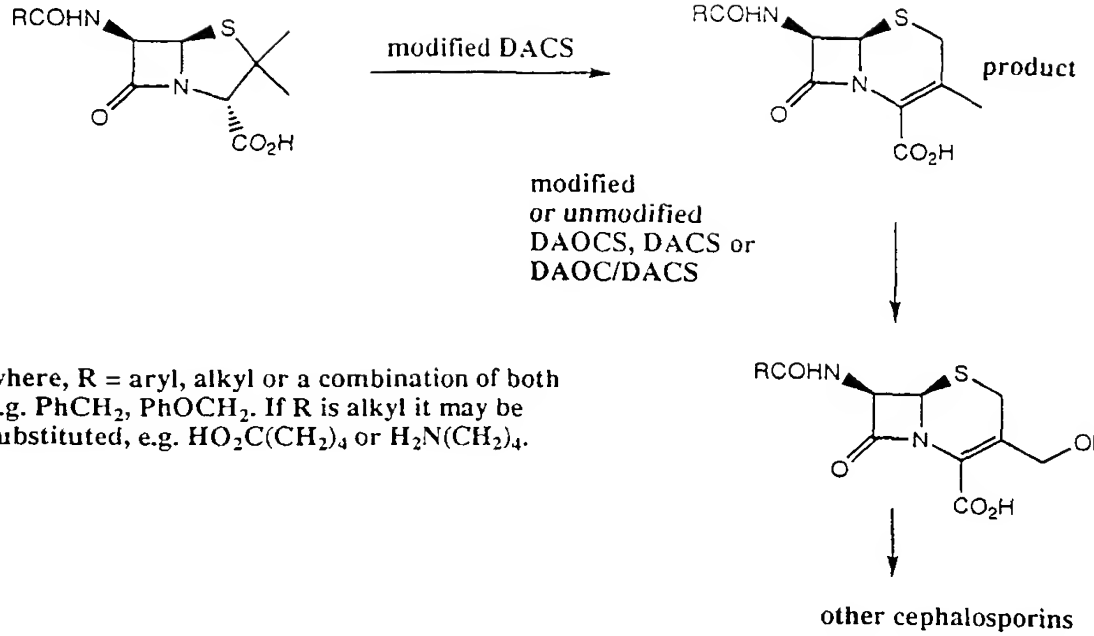
Scheme 12

example



Scheme 15

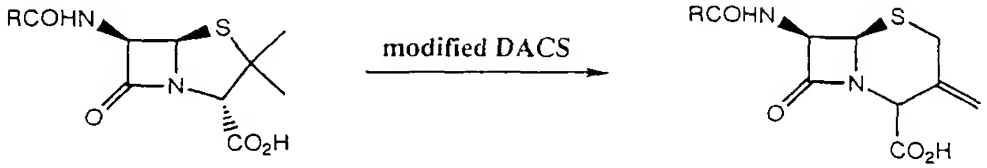
examples



where, R = aryl, alkyl or a combination of both e.g. $PhCH_2$, $PhOCH_2$. If R is alkyl it may be substituted, e.g. $HO_2C(CH_2)_4$ or $H_2N(CH_2)_4$.

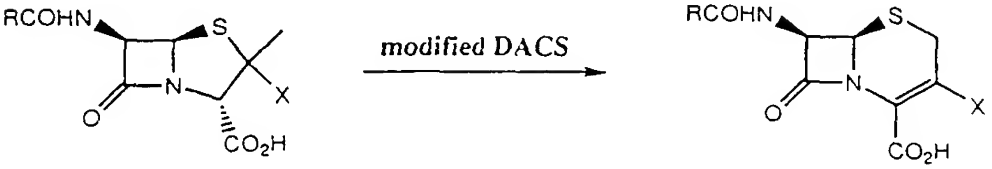
Scheme 16

example 1



where, R = D-δ-(α-aminoadipoyl), L-δ-(α-aminoadipoyl) $HO_2C(CH_2)_4$ or $H_2N(CH_2)_4$.

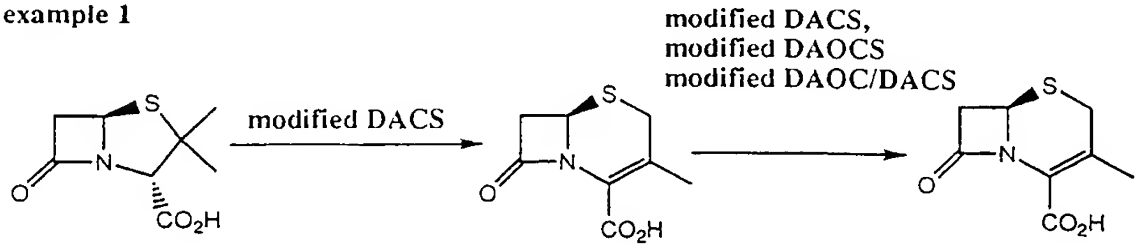
example 2



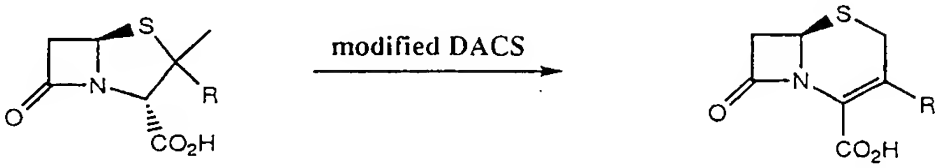
where, R = D-δ-(α-aminoadipoyl), D-δ-(α-aminoadipoyl) $HO_2C(CH_2)_4$ or $H_2N(CH_2)_4$, X = Cl, Br, I, OMe, SMe, or other substituent.

Scheme 18

example 1



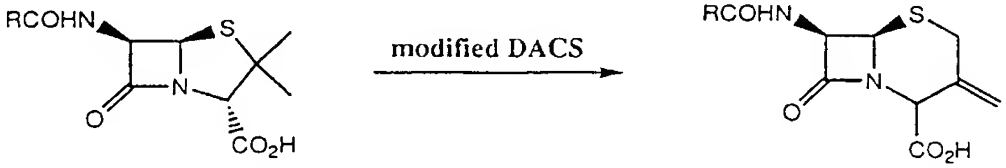
example 2



where R = Cl, Br, I, OMe or other substituent.

Scheme 19

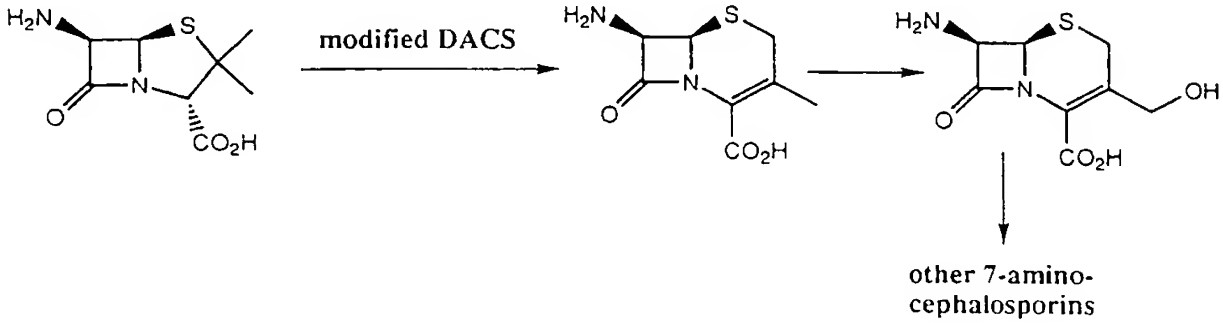
examples



where, R = aryl, alkyl or a combination of aryl and alkyl
e.g. $PhCH_2$, $PhOCH_2$.

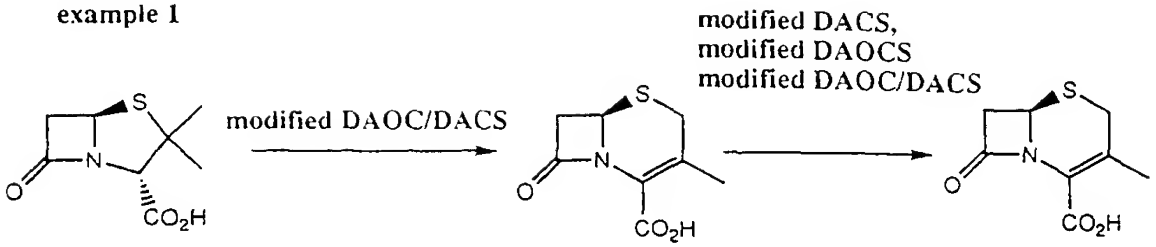
Scheme 17

example

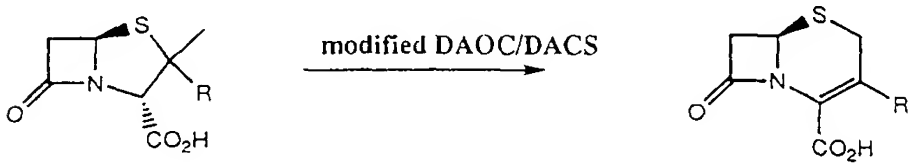


Scheme 22

example 1



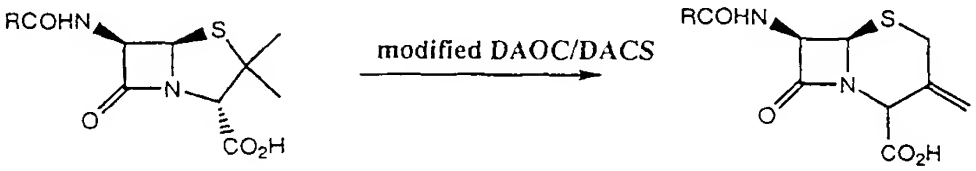
example 2



where R = Cl, Br, I, OMe or other substituent.

Scheme 23

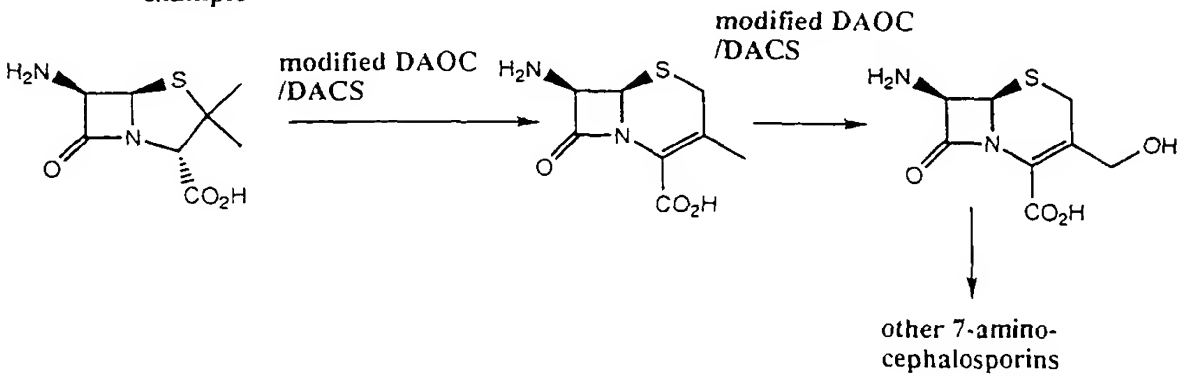
examples



where, R = aryl, alkyl or a combination of aryl and alkyl
e.g. $PhCH_2$, $PhOCH_2$.

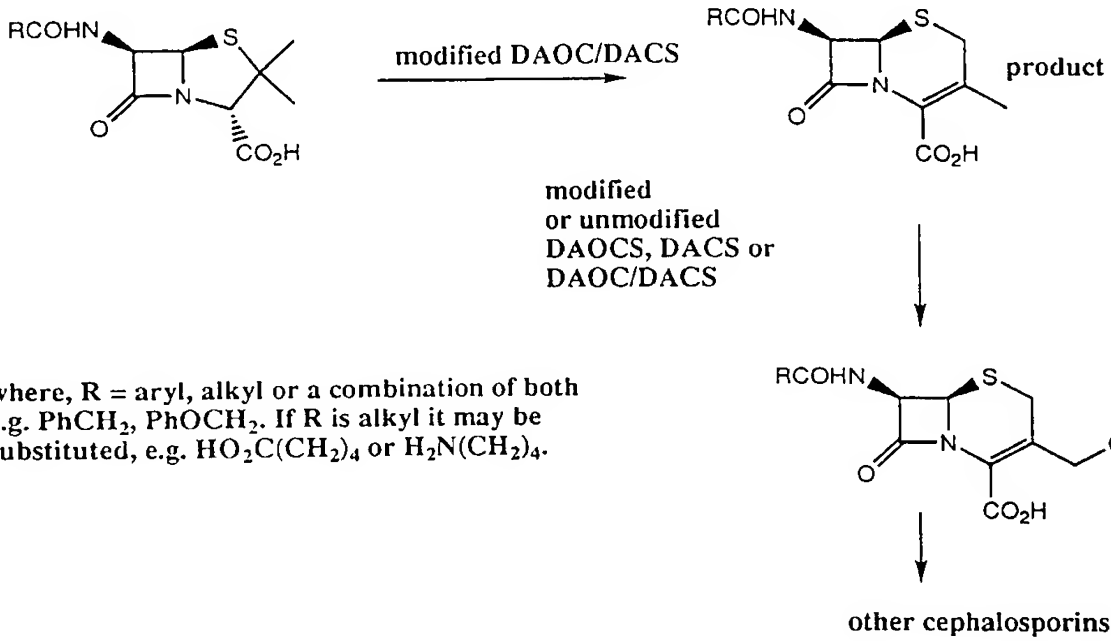
Scheme 21

example



Scheme 24

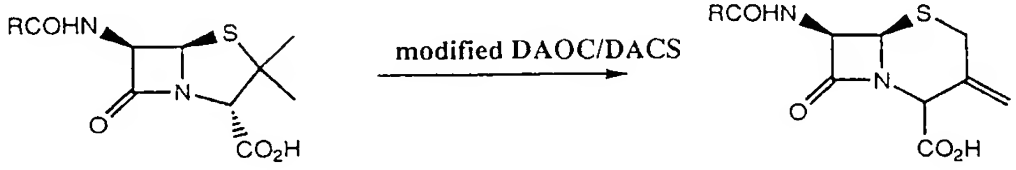
examples



where, R = aryl, alkyl or a combination of both e.g. $PhCH_2$, $PhOCH_2$. If R is alkyl it may be substituted, e.g. $HO_2C(CH_2)_4$ or $H_2N(CH_2)_4$.

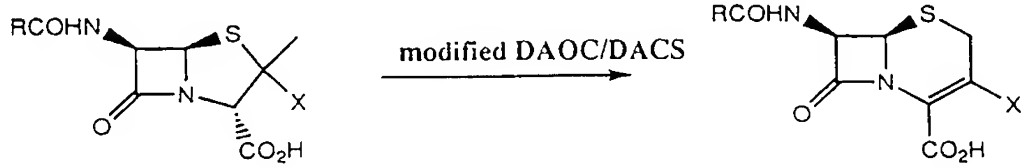
Scheme 20

example 1



where, R = D-δ-(α-aminoadipoyl), L-δ-(α-aminoadipoyl) $HO_2C(CH_2)_4$ or $H_2N(CH_2)_4$.

example 2



where, R = D-δ-(α-aminoadipoyl), D-δ-(α-aminoadipoyl) $HO_2C(CH_2)_4$ or $H_2N(CH_2)_4$, X = Cl, Br, I, OMe, SMe, or other substituent.

CLAIMS

1. Isopenicillin N synthase (IPNS) in the form of: a complex with Mn having a structure designated by the X-ray co-ordinates in Table 2; or a complex with Fe and its substrate, said complex having a structure designated by the X-ray co-ordinates in Table 3.

2. Isopenicillin N synthase (IPNS) in the form of: a complex with Fe and an analogue of its substrate, either in the absence or in the presence of nitrous oxide or dioxygen, said complex having a structure designated by X-ray co-ordinates analogous to that set out in Table 3.

3. Use of the three dimensional structure of a first enzyme selected from IPNS, DAOCS, DACS, DAOC/DACS and other related enzymes of the penicillin and cephalosporin biosynthesis pathway, for the modification of a second enzyme selected from IPNS, DAOCS, DACS, DAOC/DACS and other related enzymes of the penicillin and cephalosporin biosynthesis pathway.

4. Use as claimed in claim 3, wherein the second enzyme is modified to accept unnatural substrates for the preparation of antibacterial materials or intermediate for the production of pharmaceutical products.

5. Use as claimed in claim 3, wherein the second enzyme is modified to produce unnatural products or improve the production of natural products.

6. An enzyme having significant (as herein defined) sequence similarity to IPNS, wherein at least one of the following amino acid residues is modified:

R287; R87; R88; Y189; S183; Y91; F285; Q330; T331; V185; L106; C104; V217; L324; L317; I325; L321; S210.

7. An enzyme having significant (as herein defined) sequence similarity to IPNS, wherein at least one of the following amino acid residues is modified:

V272; L231; L223; P283; T221; F211; F285; Q330; I187; V185; Y189; R279; S281; N230; Q225; N252; S210.

8. A gene which codes for the enzyme of claim 6 or claim 7.

9. A micro-organism containing the gene of claim 8 and which is capable of expressing the gene under fermentation conditions.

10. Use of the micro-organism of claim 9 for making a bicyclic β-lactam of the penicillin or cephalosporin (including cephams) families.

11. Use of the enzyme of claim 6 or claim 7 for the preparation *in vitro* of a bicyclic β-lactam of the penicillin and cephalosporin families.

12. In a method for the preparation of an enzyme, selected from IPNS, DAOCS, DACS, DAOC/DACS and sequence-related enzymes, in crystalline form for X-ray diffraction studies, the improvement which consists in maintaining the enzyme under anaerobic conditions with dioxygen substantially absent.

13. A method which comprises using the three dimensional structure of a first enzyme selected from IPNS, DAOCS, DACS, DAOC/DACS and other related enzymes of the penicillin and cephalosporin biosynthesis pathway, for determining or predicting the structure of a second enzyme which is structurally related to the first enzyme but is not active in the penicillin or cephalosporin biosynthesis pathway, and using the structural information so obtained for modifying the second enzyme or for designing an inhibitor for the second enzyme.

14. Use of the enzyme of claim 6 or claim 7 to convert a dipeptide to a 6- aminopenicillin or other bicyclic β-lactam.

15. Use as claimed in claim 14, wherein the dipeptide has been produced by use of a peptide synthetase enzyme such as ACV synthetase optionally modified to optimise dipeptide production.

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(57) Abstract

A three–dimensional structure is described of a complex of isopenicillin N synthase (IPNS) with Fe and its substrate ACV. This structure is used to design modified enzymes IPNS, DAOCS, DACS, DAOC/DACS and other related enzymes of the penicillin and cephalosporin biosynthesis pathway, which modified enzymes may accept unnatural substrates or improve production efficiency or produce improved products. Specific modifications of specific amino acid residues are proposed and exemplified.

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INTERNATIONAL SEARCH REPORT

International Application No
PCT/GB 97/02838

A. CLASSIFICATION OF SUBJECT MATTER
IPC 6 C12N15/52 C12N9/00 C12P35/00 C12N1/21

According to International Patent Classification (IPC) or to both national classification and IPC

B. FIELDS SEARCHED

Minimum documentation searched (classification system followed by classification symbols)
IPC 6 C12N

Documentation searched other than minimum documentation to the extent that such documents are included in the fields searched

Electronic data base consulted during the international search (name of data base and, where practical, search terms used)

C. DOCUMENTS CONSIDERED TO BE RELEVANT

Category °	Citation of document, with indication, where appropriate, of the relevant passages	Relevant to claim No.
X	ROACH PL ET AL: "Crystal structure of isopenicillin N synthase is the first from a new structural family of enzymes." NATURE 375 (6533) P700-4 JUN 22 1995, XP002059796 cited in the application see abstract; figures 1-3; table 1 ---	1
X	SCOTT RA ET AL: "X-ray absorption spectroscopic studies of the high-spin iron(II) active site of isopenicillin N synthase: evidence for Fe-S interaction in the enzyme-substrate complex." BIOCHEMISTRY 31 (19) P4596-601 MAY 19 1992, XP002067783 see the whole document --- -/--	1,2

[X] Further documents are listed in the continuation of box C.

[X] Patent family members are listed in annex.

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Date of the actual completion of the international search	Date of mailing of the international search report
11 June 1998	30.06.98

Name and mailing address of the ISA	Authorized officer
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C.(Continuation) DOCUMENTS CONSIDERED TO BE RELEVANT

Category °	Citation of document, with indication, where appropriate, of the relevant passages	Relevant to claim No.
X	ORVILLE, ALLEN M. ET AL: "Thiolate ligation of the active site iron(II) of isopenicillin N synthase derives from substrate rather than endogenous cysteine: spectroscopic studies of site-specific Cys.fwdarw. Ser mutated enzymes" BIOCHEMISTRY (1992), 31(19), 4602-12 CODEN: BICHAW;ISSN: 0006-2960, XP002067784 see the whole document	1,2
X	BLACKBURN JM ET AL: "A heuristic approach to the analysis of enzymic catalysis: reaction of delta-(L-alpha-aminoadipoyl)-L-cysteinyl-D -alpha-aminobutyrate and delta-(L-alpha-aminoadipoyl)-L-cysteinyl-D -allylglycine catalyzed by isopenicillin N synthase isozymes." BIOCHEMISTRY, JUN 6 1995, 34 (22) P7548-62, UNITED STATES, XP002067785 see the whole document	1,2
X	HUFFMAN GW ET AL: "Substrate specificity of isopenicillin N synthase." J MED CHEM, MAY 15 1992, 35 (10) P1897-914, UNITED STATES, XP002067786 see the whole document	1,2
A	DATABASE BIOTECHNOLOGY ABSTRACTS DERWENT ,LONDON aN 88-01715, PRATT A J: "Manipulation of beta-lactam biosynthetic enzymes" XP002067788 see abstract & ABSTR.PAP.AM.CHEM.SOC., 1987,	6-11,14, 15
A	EP 0 307 171 A (LILLY CO ELI) 15 March 1989 see claims 1-8	1,2, 6-11,14, 15
A	EP 0 317 096 A (LILLY CO ELI) 24 May 1989 see claims 1-18	1,2, 6-11,14, 15

-/--

C.(Continuation) DOCUMENTS CONSIDERED TO BE RELEVANT

Category °	Citation of document, with indication, where appropriate, of the relevant passages	Relevant to claim No.
A	TAN, DOREEN S. H. ET AL: "Functional analysis of conserved histidine residues in Cephalosporium acremonium isopenicillin N synthase by site-directed mutagenesis" J. BIOL. CHEM. (1996), 271(2), 889-94 CODEN: JBCHA3;ISSN: 0021-9258, XP002060004 see abstract see page 889, right-hand column, paragraph 2; figures 1,4; tables 2,3 see page 893, left-hand column, paragraph 2 ---	1,2, 6-11,14, 15
A	KRIAUCIUNAS A ET AL: "The functional role of cysteines in isopenicillin N synthase. Correlation of cysteine reactivities toward sulfhydryl reagents with kinetic properties of cysteine mutants." J BIOL CHEM, JUN 25 1991, 266 (18) P11779-88, UNITED STATES, XP002060005 see abstract see page 11780, left-hand column, paragraph 3 see page 11782, right-hand column, line 12 - line 17 ---	1,2, 6-11,14, 15
P,X	SAMI, MALKIT ET AL: "Glutamine-330 is not essential for activity in isopenicillin N synthase from Aspergillus nidulans" FEBS LETT. (1997), 405(2), 191-194 CODEN: FEBLAL;ISSN: 0014-5793, XP002059797 see the whole document ---	1,6-11, 14,15
P,X	ROACH, PETER L. ET AL: "Structure of isopenicillin N synthase complexed with substrate and the mechanism of penicillin formation" NATURE (LONDON) (1997), 387(6635), 827-830 CODEN: NATUAS;ISSN: 0028-0836, XP002067787 see the whole document ---	1,2
P,X	WO 97 20053 A (GIST BROCADES BV ;UNIV OXFORD (GB); SUTHERLAND JOHN DAVID (GB); BO) 5 June 1997 see claims 1-9; figure 1 -----	6-11,14, 15

INTERNATIONAL SEARCH REPORT

national application No
PCT/GB 97/02838

Box I Observations where certain claims were found unsearchable (Continuation of item 1 of first sheet)

This International Search Report has not been established in respect of certain claims under Article 17(2)(a) for the following reasons:

1. ☐ Claims Nos.:
because they relate to subject matter not required to be searched by this Authority, namely:

2. ☐ Claims Nos.:
because they relate to parts of the International Application that do not comply with the prescribed requirements to such an extent that no meaningful International Search can be carried out, specifically:

3. ☐ Claims Nos.:
because they are dependent claims and are not drafted in accordance with the second and third sentences of Rule 6.4(a).

Box II Observations where unity of invention is lacking (Continuation of item 2 of first sheet)

This International Searching Authority found multiple inventions in this international application, as follows:

see additional sheet

1. ☐ As all required additional search fees were timely paid by the applicant, this International Search Report covers all searchable claims.

2. ☐ As all searchable claims could be searched without effort justifying an additional fee, this Authority did not invite payment of any additional fee.

3. ☒ As only some of the required additional search fees were timely paid by the applicant, this International Search Report covers only those claims for which fees were paid, specifically claims Nos.:

1 2 6-11 14 15

4. ☐ No required additional search fees were timely paid by the applicant. Consequently, this International Search Report is restricted to the invention first mentioned in the claims; it is covered by claims Nos.:

Remark on Protest

☐ The additional search fees were accompanied by the applicant's protest.

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INTERNATIONAL SEARCH REPORT

International Application No. PCT/GB 97/02838

FURTHER INFORMATION CONTINUED FROM PCT/ISA/ 210

This International Searching Authority found multiple (groups of) inventions in this international application, as follows:

1. Claim : 1 partly

   IPNS complexed with Mn

2. Claim : 2 and 1 partly

   IPNS complexed with Fe and ist substrate or an analogue of its substrate

3. Claims: 3-5 , 13

   the use of the three dimensional structure of a member of the IPNS family of enzymes to modify another enzyme .

4. Claims: 6-11,14-15

   Enzyme having significant sequence similarity to IPNS wherein at least one of the following amino acid residues is modified ,r87,y189,s183,y91,f285,q330,t331 v185,l106,c104,v217,l324,l317,i325,l321,s210,v272,l231, l223,p283,t221,f211,i187,v185,y189,r279,s281,n230,q225,n252, r287,r88, mutants of an enzyme having similarity to IPNS , gene encoding it , micro-organism containing the gene and their use in beta-lactam production .

5. Claim : 12

   methods of preparation of an enzyme of the IPNS family in crystalline form consisting of maintaining the crystalline enzymes of the IPNS family under anaeorobic conditions .

INTERNATIONAL SEARCH REPORT

Information on patent family members

International Application No
PCT/GB 97/02838

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